The Area of Contact for Non-Adhesive Rough Surfaces

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Abstract Book

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Plenary

(plenary) **Model-reduction in multiscale problems for composite and polycrystalline materials**

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A common practice in multiscale problems for heterogeneous materials with well separated scales, is to look for homogenized, or effective, constitutive relations. In linear elasticity the structure of the homogenized constitutive relations is strictly preserved in the change of scales. The linear effective properties can be computed once for all by solving a finite number of unit-cell problems.

Unfortunately there is no exact scale-decoupling in multiscale nonlinear problems which would allow one to solve only a few unit-cell problems and then use them subsequently at a larger scale. Computational approaches developed to investigate the response of representative volume elements along specific loading paths, do not provide constitutive relations. Most of the huge body of information generated in the course of these costly computations is often lost.

Model reduction techniques, such as the Non Uniform Transformation Field Analysis ([1]), may be used to exploit the information generated along such computations and, at the same time, to account for the commonly observed patterning of the local plastic strain field. A new version of the model [2] will be proposed in this talk, with the aim of preserving the underlying variational structure of the constitutive relations (similar objective in [3]), while using approximations which are common in nonlinear homogenization.

[1] J.C. Michel, P. Suquet, Int. J. Solids Structures 40, 6937-6955 (2003)
[2] J.C. Michel, P. Suquet, J. Mech. Phys. Solids, In press (2016)
[3] F. Fritzen, M. Leuschner, Comput. Meth. Appl. Mech. Eng. 260, 143–154 (2013)

(plenary) **The effect of dislocation junctions on the work hardening rate of face-centered cubic metals**

W Cai[1], R B Sills[2,1], A Aghaei[1] and N Bertin[1]

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Understanding plasticity and strength of crystalline materials in terms of the physics of microscopic defects has been a long-standing goal of materials research. Over the last two decades, much effort has been placed on the prediction of stress-strain curve of single crystals through large-scale dislocation dynamics (DD) simulations. If successful, DD can thus provide a quantitative link, which has been lacking to date, between dislocation physics at the atomistic scale and crystal plasticity at the continuum scale. Unfortunately, the progress in this direction has been limited by the very small strain that can be routinely reached (<1%) by existing DD simulations compared with the typical strain (up to 30%) in experiments. Because of this limitation, a direct comparison between DD predictions and experimental stress-strain curves has been impossible.

A series of advanced time integration algorithms have been developed to expand the strain range of DD simulations [1]. In particular, the pairwise interaction forces between dislocation segments are separated into several groups, and each group is integrated with a different time step size. The resulting (force-based subcycling) algorithm leads to an increase of computational efficiency by more than 100 times. The new simulation capability enables the prediction of stress-strain curves for shear strains in excess of 1% routinely and repeatedly. As a result, a systematic investigation on the relation between the unit mechanisms and work hardening rate is now possible.

The strain hardening rates predicted by DD simulations in FCC metals under [001] loading are consistent with stage II of the quasi-static stress-strain response observed in experiments, i.e. on the order of μ/200 [2]. By changing rules on unit mechanisms in DD simulations, we determine the relative importance of different dislocation reactions on the hardening rate. We find that glissile junctions are the most important junction type for hardening, with collinear and Lomer junctions second most important. Interestingly, the relative importance of different junctions in hardening is not the same as that in strength. A Boltzmann-type theory based on dislocation line length distributions is constructed to explain the role of different junctions on the hardening rate revealed by DD simulations.

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[1] R. B. Sills, A. Aghaei, and W. Cai, Advanced Time Integration Algorithms for Dislocation Dynamics Simulations of Work Hardening, Submitted to Modelling Simul. Mater. Sci. Eng. (2015)

[2] U. F. Kocks and H. Mecking, Physics and phenology of strain hardening: the FCC case, Prog. Materials Science, 48, 171-273 (2003)

(plenary) **Can a simulation be reality? Does it matter?**

H Van Swygenhoven-Moens

Paul Scherrer Institut & EPFL, Switzerland

Synergies between experiment and multiscale materials modelling are since many years a booming topic in science, with both communities stimulating each other. This can be ascribed to a great extend to an increasing availability of high performance computing resources. These resources have allowed the development of simulations over a large span of length and time scales. One should however recognize that the increase in computational capacities has also allowed further developments in experimental techniques and data analysis.

In science simulations can be used to mimic “experiments” on a model system with the aim to understand the outcome of an experiment. In such cases one tries to make the model as close as possible to reality. However more and more research is devoted to the development of computational tools allowing to turn-on or switch-off physical mechanisms in order to distinguish between essential and incidental mechanisms among all what is possibly occurring in real life. In these simulations the model simulated is usually further away from reality. Mechanistic insights provided have then the potential to develop predictive computational tools and to design new experiments with validating character.

By using illustrative examples involving different length and time scales we will elaborate how experiments stimulate the simulation world and how simulations stimulate experimental research with an outlook to the future.

(plenary) **Reaching experimental times at the atomic scale in complex materials: the kinetic activation-relaxation technique**

N Mousseau

Université de Montréal, Canada

In spite of considerable advances in computational capacities over the last decades, there remains a considerable gap between experimentally relevant time scales and those accessible to atomistic simulations. This gap reflects the fundamentally multi scale nature of atomistic kinetics that can only be lifted partially through approximate methods that attempt to capture the most important aspect of specific phenomena. Among those approaches, the kinetic activation-relaxation technique (k-ART) is an off-lattice kinetic Monte Carlo with on-the-fly cataloging capabilities that allows fully atomistic second-long and more simulations of complex alloys and amorphous systems such as amorphous silicon and steels, while incorporating exactly elastic effects. In this talk, I'll present the k-ART method, recent applications to various systems and its advantages and limitations in the study of complex materials.

(plenary) **Data-driven materials research: Novel routes to new insight and predictions**

C Draxl

Humboldt-Universität zu Berlin and Fritz Haber Institute of the Max Planck Society, Germany

On the steady search for advanced materials with tailored properties and novel functions, high-throughput screening has become a new branch of materials research. For successfully exploring the chemical compound space from a computational point of view, two aspects are crucial. These are reliable methodologies to accurately describe all relevant properties for all materials on the same footing, and new concepts for getting insight into the materials data that are produced since many years with an exponential growth rate.

What are our concepts for tackling big data of materials science? It is not an issue of boosting more high-throughput calculations but it is about the question: How to exploit the wealth of information, inherently inside the materials data which promises unprecedented insight?

I will first introduce the NoMaD Repository [1], which was established to promote the idea of open access and sharing of materials data. As open access implies that data can be used by anyone, large collections of materials data opens an avenue for using and developing tools that the present (computational-)materials community does not even know. The latter is now being realized in the Novel Materials Discovery Laboratory – a European Center of Excellene [2]. Here the main aims are the creation of a Materials Encyclopedia and the development of big-data analytics tools for materials science. Finally, I will demonstrate some examples how statistical-learning approaches based on domain-specific knowledge can indeed lead to new scientific insight [3].

[1] The Novel Materials Discovery (NoMaD) Repository: https://nomad-repository.eu
[2] NOMAD Center of Excellence, funded by the EU within HORIZON2020: http://nomad-CoE.eu
[3] L. Ghiringhelli, J. Vybiral, S. V. Levchenko, C. Draxl, and M. Scheffler, Big Data of Materials Science - Critical Role of the Descriptor, Phys. Rev. Lett. 114, 105503 (2015)

(plenary) **Computational mechanics in advancing the Integrated Computational Materials Science & Engineering (ICMSE) initiative for metals and alloys**

S Ghosh

Johns Hopkins University, USA

The Integrated Computational Materials Science & Engineering or ICMSE initiative entails integration of information across length and time scales for materials phenomena. This talk will present an integration of methods in Computational Mechanics and Computational Materials Science to address the deformation and failure characteristics of polycrystalline metals in various applications. Specifically it will address physics based modeling at different scales and multi-scale spatial (scale-bridging) and temporal modeling methods for Titanium, Magnesium and Aluminum alloys and Nickel based-superalloys. Spatial scales will range from atomistic to component levels. Application domains will include both monotonic and cyclic loading and address properties such as time and location-dependent strength, ductility and fatigue life. The talk will begin with methods of 3D virtual image construction and development of statistically equivalent representative volume element at multiple scales. Subsequently it will discuss the development of novel system of experimentally validated physics-based crystal plasticity finite element or CPFE models to predict deformation and micro-twinning leading to crack nucleation. These CPFE simulations will provide a platform for the implementation of physics-based crack evolution criterion that accounts for microstructural inhomogeneity. For crack evolution, a coupled molecular dynamics-continuum model for a crystalline material with an embedded crack will be discussed. A wavelet transformation based multi-time scaling (WATMUS) algorithm for accelerated crystal plasticity finite element simulations will be discussed as well. The method significantly enhances computational efficiency in comparison with conventional single time scale integration methods. Finally, stabilized element technology for analyzing this class of complex deformation problems will be discussed.

(plenary) **Crystallography in Curved Space - the Interplay of Crystalline Order, Geometry and Topology**

A Voigt

Technische Universität Dresden, Germany

The ground state configurations of two-dimensional crystals fully covering a curved surface are not defect free. Due to topological reasons they feature crystalline defects, such as disclinations, dislocations, grain boundary scars and pleats. What determines the type of defects? How do geometric properties influence their locations? Can these ground states be accessed under growth? Is our understanding for crystalline defects also useful for defects in liquid crystals on curved surfaces? We will answer these questions by phase-field-crystal simulations. The modeling approach will be introduced and discussed in detail together with appropriate numerical schemes.

(plenary) **A new simulator for real-scale dislocation plasticity based on dynamics of dislocation-density functions**

A Ngan and M H S Leung

University of Hong Kong, Hong Kong

Current strategies of computational crystal plasticity that focus on individual atoms or dislocations are impractical for real-scale, large-strain problems even with today's computing power. Dislocation-density based approaches are a way forward but most schemes published to-date give a heavier weight on the consideration of geometrically necessary dislocations (GNDs), while statistically stored dislocations (SSDs) are either ignored or treated in ad hoc manners. In reality, however, the motions of GNDs and SSDs are intricately linked through their mutual (e.g. Taylor) interactions. A correct scheme for dislocation dynamics should therefore be an "all-dislocation" treatment that is equally applicable for all dislocations, with a rigorous description of the interactions between them.

In this talk, a new formulation for computational dynamics of dislocation-density functions, based on the above "all-dislocation" principle, is discussed. The dynamic evolution laws for the dislocation densities are derived by coarse-graining the individual density vector fields of all the discrete dislocation lines in the system, without distinguishing between GNDs and SSDs. Elastic interactions between dislocations in 3D are treated in full in accordance with Mura's formulation for eigen stress. Dislocation generation is considered as a consequence of dislocations to maintain their connectivity, and a special scheme is devised for this purpose. The model is applied to simulate a number of intensive microstructures involving discrete dislocation events, including loop expansion and shrinkage under applied and self stress, dipole annihilation, and Orowan looping. The scheme can also handle high densities of dislocations present in extensive microstructures.

(plenary) **Size effects in fracture and plasticity**

Stefano Zapperi

University of Milan, Italy

The size dependence of strength is a well known but still unresolved issue in the fracture of materials and structures. The difficulty in addressing this problem stems from the complex interplay between microstructual heterogeneity and long-range elastic interactions. Furthermore, in micro and nanoscale samples, the plastic yield strength displays size effects and strain bursts, features that are not present in macroscopic samples where plasticity is a smooth process. Large fluctuations both in fracture processes and in microscale plasticity make the use of conventional continuum mechanics problematic and calls instead for a statistically based approach. In this talk, I will review recent results obtained from idelized models of disordered fracture and from more realistic simulations of defected graphene. Finally, I will discuss the size dependence of strain burst statistics as revealed by statistical models for crystal and amorphous plasticity.

(plenary) **Programming shape**

L Mahadevan

Harvard University, USA

Recent progress in understanding the shape-shifting abilities of thin sheets and slender filaments in natural (morphogenetic) and artificial (engineered) settings naturally raises the prospect that we might be able to design and control shape for function at multiple scales. I will describe our attempts to solve this inverse problem that combines geometry, matter and motion in the context of controlled precipitation for functional nanoscale structures, phytomimetic 4D printing of stimulus-responsive structures, inverse origami for programming curvature, and inverse design of active filaments for optimal locomotion.

Symposium A

(A1 invited) **Designing the mechanical response of additively manufactured silicone cellular solids with ordered porous architectures**

T Weisgraber, E Duoss, J Lewicki, A Maiti, W Small, C Spadaccini, T Wilson and R Maxwell

Lawrence Livermore National Laboratory, USA

Traditional stochastic foams are widely used for impact mitigation and static load distribution, but their designs are limited to bulk properties without the ability to control local variation. These qualities restrict the ability to develop predictive stress responses and aging models for these materials. Direct ink writing (DIW), a 3D additive manufacturing processes, produces ordered architectures, allowing a robust geometry-based design for specified anisotropic and inhomogeneous behaviour. Moreover, properties such as porosity and stiffness can be decoupled and localized. Both mechanical testing and finite element analysis provides the opportunity to explore the structure-property relationship of these cellular solids with micro-scale continuum features. In addition, structural details obtained from X-ray computed tomography inform the parametric finite element "as-built" design models with knowledge of the DIW process. Here, we present experimentally validated simulation results for a variety of 3D printed porous architectures to highlight the range of mechanical response available from these structures. A general hyperelastic foam model, with architecture dependent material parameters, is also introduced to enhance optimization in cushioning applications.

(A1 oral) **An ICME approach for additive manufacturing**

J Belak[1], J Turner[2], W King[1], N Carlson[3], N Henson[3], T Blacker[4] and L Levine[5]

[1]Lawrence Livermore National Laboratory, USA, [2]Oak Ridge National Laboratory, USA, [3]Los Alamos National Lab, USA, [4]Sandia National Lab, USA, [5]National Institute of Standards and Technology, USA

Additive manufacturing (AM) offers the prospect of revolutionizing the fabrication of components and parts with unique properties such as lightweight strength and component integration to avoid failures at joints and welds. AM is about making new parts a new way, not old parts a new way. Despite this enormous potential, the insertion of AM parts has been limited due to the difficulty in qualifying parts. Starting from a top->down systems engineering approach, an integrated computational materials engineering (ICME) approach can be used to accelerate the qualification and adoption of newly additively manufactured parts. The AM process is unique in that the component is created directly from the CAD drawing of the design specification by the addition of small two-dimensional layers. The ICME process uses optimization across all levels from performance to fabrication to create an optimal design specification with margins that fully incorporates the application design requirements and the variabilities in the build process, including residual stress and local material properties. Three-dimensional x-ray diffraction (3DXRD) tomography coupled with the emerging generation of extreme-scale computing offers a particular interesting paradigm to quantify local material properties by non-destructive characterization of 3D microstructures that are input to high fidelity simulations so that the simulation and the material test experiment are performed on the same initial microstructure. Here we present a detailed analysis of this process for the use-case of metal additive manufacturing.

(A1 oral) **Multiscale optimization for novel material design using a combined numerical and experimental approach**

G Gu, L Dimas, Z Qin and M Buehler

Massachusetts Institute of Technology, USA

Materials of the future will be stronger, smarter, tougher, lighter, and more sustainable. Natural materials are the key to unleashing the potential of materials that can adapt to environmental changes such as employing self-healing processes, protecting against predators, and changing skin colors. However, most engineering materials today do not possess the hierarchical architectures and multifunctionality seen in nature. In our work, we postulate that we can use nature's design tools to tune and optimize for specific mechanical properties such as toughness and strength to improve synthetic materials. Here we employ an optimization algorithm to explore and design composites using soft and stiff building blocks to study the underlying mechanisms of nature's tough materials. Our goal is to use this building block and optimize it across scales by manipulating the grouping and arrangement of these blocks to achieve an architectured flaw tolerant composite. Furthermore, because our designs involve multiple materials organized in diverse geometries, we use multi-material 3D-printing to overcome manufacturing limitations inherent in traditional subtractive manufacturing. Our results show that an algorithmic design coupled with 3D-printing technology and experimental mechanical testing using digital image correlation can generate morphologies with tougher and stronger than the strongest base material. This provides a proof of concept that through multiscale computational modeling, complementary material properties can be designed and optimized to synthesize biomimetic composites that are more efficient and fracture resistant.

(A1 oral) **Mechanical and morphological study of dental tissues**

E Vennat[1], W Wang[1], T Reiss[1], E Dursun[2], A Gourrier[3] and J-M Allain[4]

[1]Centrale-Supélec, France, [2]University Paris Descartes, France, [3]University Joseph Fourier, France, [4]Ecole Polytechnique, France

In order to overcome the lack of durability of dentinal restorations, it is crucial to understand the multi-scale mechanical behaviour of the sound and restored dental tissues to provide optimized restoration protocols and new techniques or restorative materials. Here, dentin, which is the bulk material of tooth, is investigated to complete the knowledge of its three-dimensional microstructure. The local microstructure are observed and quantified using:

- Confocal microscopy for three-dimensional characterization of the porous network;
- Focused Ion Beam-Scanning electron microscopy for tubules, peritubular dentin and intertubular dentin 3D representation;
- Atomic force microscopy (AFM) for local mechanical properties and 2D topology assessment.

At the upper scale, dentin tissue mechanical elastic properties are assessed and linked to the lower scale investigations. Compression tests are carried out under microscope in order to get the strain field using Digital Image Correlation and the Finite Element Method is used to have the stress field.

The findings from this study will then be used to model the restored tooth at the organ scale.

(A2 invited) **Optimal design and advanced manufacturing of micro and nano-architected materials**

L Valdevit

University of California, Irvine, USA

Architected cellular materials (i.e., single or multi-phase periodic cellular materials with unit cell topology optimized for one or more functionalities) have been extensively investigated over the past two decades, for their potential to achieve combinations of properties unavailable in any existing monolithic material. More recently, exceptional advances in additive manufacturing technologies have enabled fabrication of macro-scale architected materials with key dimensional features at the micro and nanoscale. As mechanical properties of materials often exhibit beneficial size effects at the nanoscale (e.g., strengthening of metals and toughening of ceramics), these fabrication approaches provide a unique opportunity to translate these beneficial effects to a macro-scale structural or multifunctional material with unique combinations of properties, such as exceptional strength and low weight under very high (or very low) temperatures and aggressive environmental conditions, fully elastic recovery from very large strains, zero (or negative) coefficient of thermal expansion, shape morphing capabilities, unique combinations of stiffness and damping, and many other unusual characteristics. Two key challenges that limit the practical implementation of micro/nano architected materials are (i) the development of scalable multi-material, multiscale manufacturing processes suitable for production of highly hierarchical cellular materials; and (ii) the development of modelling and design tools to identify the optimal cellular topology to translate nanoscale benefits into excellent macroscale properties. In this talk, I will present some of our recent efforts towards the fabrication, modelling, characterization and optimal design of a number of micro/nano-architected materials optimized for high strength, stiffness, toughness and energy dissipation at very low density.

(A2 oral) **Homogenized dynamics of lattice-structured meta-materials**

M Messner, J Moore and N Barton

Lawrence Livermore National Laboratory, USA

Additively manufactured lattice meta-materials have complex dynamics, including the attenuation and dispersion of elastic waves and the possibility of acoustic bandgaps. A homogenized model embedding the dynamics of these materials into conventional finite element simulations requires microinertial corrections accounting for these complex dynamic effects. This presentation describes a model accounting for microinertial effects in the limit of long wavelengths. Depending on the approximations made, the difficulty of implementing the microinertial correction ranges from simply changing the effective density of the material to altering the process used to calculate the inertial body force. The presentation describes the accuracy of various microinertial approximations as well as makes comparisons between fully resolved simulations of lattice materials and their homogenized equivalents.

(A2 oral) **Crystal plasticity study of monocrystalline stochastic honeycombs under in-plane compression**

F Roters[1], D Ma[1], P Eisenlohr[2], P Shanthraj[1], M Diehl[1] and D Raabe[1]

[1]MPI für Eisenforschung, Germany, [2]Michigan State University, USA

We present a crystal plasticity study on the plastic deformation of single crystalline stochastic honeycombs under in-plane compression, focusing on the very early stage of plastic deformation. Detailed comparison is made between the single crystalline stochastic honeycombs and the corresponding bulk single crystals in terms of the slip system activation, the mechanical anisotropy, the stress distribution, and the crystallographic reorientation. The interplay between the crystallographic orientation and the cellular structure during plastic deformation is revealed through these comparisons.

(A2 oral) **Disordered auxetic materials**

C Petersen[1], M Alava[1] and S Zapperi[2]

[1]Aalto University, Finland, [2]Università degli Studi di Milano, Italy

Auxetic materials, those with a negative Poisson ratio, have the counter-intuitive behaviour of expanding laterally when stretched longitudinally. Porous solids, such as polymer or metallic foams, are examples of man made auxetic materials. These architected materials are designed with a re-entrant cell structure. Simple two dimensional models with re-entrant geometries have successfully reproduced this auxetic behaviour. While typical auxetic materials are disordered, most theoretical and computational studies to date have been limited to ordered structures. We have computationally modeled simple disordered lattices and related their nanoscale properties, such as spring constants and geometries, to the Poisson ratio. We find that many simple geometries can be made auxetic if the lattice has stiff angular springs, relative of the stiffness of the bonds. In architected lattices with re-entrant geometries, based off those used in previous studies of ordered auxetic materials, the opposite trend is seen. We present a new disordered version of this lattice, whose Poisson ratio exhibits the same behaviour.

(A2 oral) **General properties and upper bound estimates for plasticity in porous continua**

A Benzerga[1] and J-B Leblond[2]

[1]Texas A&M University, USA, [2]Paris-Sorbonne University, France

Problems of the stressing and deformation of porous continua are ubiquitous in materials science, geophysics, civil engineering and biomechanics. Laying emphasis on elastoplastic solids with pressure-free pores, some general properties of the plastic flow behaviour of a porous continuum are presented using nonlinear homogenization and limit analysis theories. Such results are relevant to progressively cavitating solids, as would arise in problems of ductile fracture of metals and polymers, and to highly porous materials, such as cellular solids. For illustration, the emergent behaviour will be discussed under two circumstances. First, the effect of an assumed microscale plastic flow anisotropy on the enlargement of cavities in the near-dilute limit is demonstrated. Next, the influence of plastic flow concentration at the microscale on effective behaviour is discussed for large porosity levels. In perspective, a unified framework for representing seamless transitions between diffuse and localized flow is described.

(A3 invited) **Poisson's function of single-wire entangled materials: from below 0 in tension to above 0.5 in compression**

D Rodney[1] and L Orgéas[2]

[1]University of Lyon, France, [2]Grenoble INP, France

The mechanics of fibrous materials is both complex and intriguing. Here, we explore one class of such materials, made of the disordered entanglement of a single long coiled fiber. This architected material is of both fundamental and technological interests. Fundamentally, this system can be seen as a disordered material, akin to glasses, but with very long (possibly infinitely) ranged correlations transmitted along the single fiber. For applications, it is a potential replacement for sintered materials but with a very large deformability.

We study the mechanics of this material using a combination of experiments and simulations. Experimentally, we produced samples from single fibers made of either a superelastic shape-memory alloy, a viscoelastic polymer or a ductile metal. The samples were subjected to deformation cycles, tracking local deformations with optical cameras and x-ray tomography. Numerically, we employed Kirchhoff's elastic rod theory to simulate mechanical cycles on both numerical substitutes of the experimental samples and on idealized periodic samples.

This architecture exhibits surprising mechanical properties, partly because of its topology in-between a discrete and a continuum medium. In particular, we find large and reversible extensions of its volume, both in tension and compression. This material is thus reversibly dilatant in both directions, with a Poisson's function varying from above 1/2 in compression to less than 0 in tension. This unusual behavior arises from an interplay between the elongation of the coiled wire and rearrangements due to steric effects, which, unlike in traditional discrete media, are reversible when the fiber is elastic.

(A3 oral) **Microstructure modeling of porous electrodes for solid oxide fuel cells (SOFCs)**

J Joos[1], T Carraro[2], H Geisler[1], A Weber[1] and E Ivers-Tiffée[1]

[1]Karlsruhe Institute of Technology (KIT), Germany, [2]Heidelberg University, Germany

Microstructure modelling of porous electrodes for solid oxide fuel cells (SOFCs) has rapidly developed over the last years. Advanced imaging techniques such as focused ion beam/scanning electron microscopy (FIB/SEM) tomography support this progress by enabling 3D reconstructions of µm- and sub-µm-scaled multiphase electrodes [1,2]. From these reconstructions microstructural parameters can be determined which form the basis for calculating electrode performance via homogenized microstructure models [2,3].

Even more desirable is a direct use the 3D FIB/SEM data in adequate performance models [3]. Therefore a 3D finite element method (FEM) model is presented, which calculates e.g. the area specific resistance (a performance index) of mixed ionic-electronic conducting cathodes by directly using the preprocessed 3D FIB/SEM data. The required size of the reconstructed volume (the computational domain in the model) and the resolution of the 3D image data are investigated. A too small volume or a not accurately resolved structure leads to untrustworthy results. In contrast, large volumes which are highly resolved demand for high computational effort, notably enormous demands for memory and long computing times.

Model calculations were validated with experimental results obtained by electrochemical impedance spectroscopy. Combining experimental and modelling results is the key to predict cathode characteristics as a function of operating conditions and material configurations and thus enables a well-directed improvement of the SOFC performance.

[1] J.R. Wilson, et al., Nature Materials 5 (17), p. 541 (2006)
[2] J. Joos, et al., Electrochim. Acta 82, p. 268 (2012)
[3] T. Carraro, et al., Electrochim. Acta 77, p. 315 (2012)

(A3 oral) **Size effects and irregularity in open cellular foams**

S Liebenstein, S Sandfeld and M Zaiser

Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Open cellular foams are lightweight materials common in nature (e.g. cork or cancellous bone) and as man-made structures (e.g. metal and polymer foams). They exhibit good weight specific properties, i.e. bending stiffness, energy absorption and thermal insulation. The microstructure can be described as a network of struts or beams and its related characteristic length, i.e. bond length or cell size is a result of the forming process and therefore independent of the system size. As a result geometrically similar systems of different size behave differently. These size effects can be observed experimentally [1], but also in simulations.

Often the microstructure is of random nature, so that it is of special interest to understand the interplay between size dependant mechanical behaviour and irregularity. For a statistical analysis of such random systems a sufficiently large number of simulations is necessary. An efficient simulation method for modelling open cellular foams is the representation as a network of Timoshenko beams. The microstructure is automatically generated via Voronoi tesselation, which allows us to study large numbers of random systems. We show for different loading cases how size effects are influenced by local and global irregularities and how they interact with geometrical properties as e.g. the aspect ratio. In order to identify strong and weak structures a novel continuization method is presented, which allows to visualize and analyse local stress and strain patterns in a continuum sense.

[1] Andrews et. al. [1999]. Material Science and Engineering, A 270, pp. 113-124.

(A3 oral) **Elaboration of BN membrane using a new elegant approach**

C Marichy, V Salles and A Brioude

Laboratory of Multimaterial and Interfaces - UMR 5615, France

Boron nitride structures are very attractive materials with application in various areas such as the energy and the environmental domains. Recently, BN nanotubes have proven to be suited for conversion of osmotic energy.[1] Use of nanotubes arrays or membrane would thus allow osmotic power harvesting under salinity gradients. In the present work, it will be shown how it is possible to prepare a thin material containing several thousands of BN tubes, from a commercially available membrane. Using a double inversion of a polymer membrane combining atomic layer deposition and polymer derived ceramic route, good quality and large surface boron nitride membranes were elaborated. Briefly, commercial polycarbonate membrane was infiltrated at low temperature with zinc oxide using atomic layer deposition. A subsequent heat treatment permitted obtaining arrays of ZnO hollow tubes/rods by removal of the polymer scaffold. Then exposition to borazine vapor for several days leads to the conformal infiltration of the self-supported ZnO aligned nanotubes with BN-based polymer. Conversion into pure boron nitride and removal of the ZnO scaffold were realized in one single annealing step under nitrogen at high temperature. Thanks to gentle infiltration conditions, the initial structure is well-preserved without appearance of significant cracks despite the multiple steps. Good quality boron nitride membrane was then obtained, which is certainly of interest for osmotic energy application.

[1] A. Siria, P. Poncharal, A.-L Biance, R. Fulcrand, X. Blase, S. T. Purcell and L. Bocquet, Nature, 2013, 494, 455–458

(A4 invited) **Structural and mechanical inhomogeneities in cement paste**

K Ioannidou[1], E Del Gado[2], F-J Ulm[1], P Levitz[3] and R Pellenq[1]

[1]Massachusetts Institute of Technology, USA, [2]Georgetown University, USA, [3]PHENIX, CNRS and University Pierre et Marie Curie, France

Strength and other mechanical properties of cement paste and concrete rely upon the formation of Calcium–Silicate–Hydrates (C–S–H) during cement hydration. Controlling the structure and properties of the C–S–H phase is still a challenge, due to the complexity of this hydration product and of the mechanisms that drive its precipitation from the ionic solution upon dissolution of cement grains in water. Here we present a novel description of the C–S–H meso-scale texture that offers an opportunity to translate results from the fundamental scales to the macro-scale of engineering properties. We use simulations that combine information of the nano-scale building units of C–S–H and on their effective interactions, obtained from atomistic simulations and experiments, into a statistical physics framework for aggregating nanoparticles. We compute small angle scattering intensities, pore size distributions, specific surface area, local densities, indentation modulus and hardness of the material, providing a new quantitative understanding of different experimental investigations. Moreover we correlate the structural quantities with local stresses analysis to provide insight on the fracture of cement. Our results lead to a quantitative insight into how the heterogeneities developed during the early stages of hydration persist in the structure of C–S–H and impact the mechanical performance of the hardened cement paste.

(A4 oral) **Kinetic Monte Carlo simulations of nanoparticle precipitation: the early hydration rate of cement**

E Masoero and I Shvab

Newcastle University, UK

The early hydration of cement is largely controlled by the precipitation of calcium-silicate-hydrate (C-S-H) from ionic aqueous solution. Mesoscale simulations based on random nucleation and aggregation of nanoparticles can partly capture this process and relate it to the sub-micrometre texture development of the C-S-H. However, recent results from top-down chemical kinetic theory indicate that the concentration of ions in solution becomes a preeminent controlling factor, at least after 5-10 hours of hydration. The current nanoparticle simulations cannot address this regime directly because of the large timescale involved and because they do not account quantitatively for the solution chemistry. Here we propose an alternative approach, based on Kinetic Monte Carlo simulations, to overcome this limitation. The rates of nanoparticle nucleation in this approach are derived using Transition State Theory and thermodynamics (which bring the solution chemistry into the model) and considering also the free energy contributions from mechanical interactions between particles. Our results capture the experimentally measured rate of reaction during the first 24 hours of hydration, without invoking space filling and pointing to the same mechanism suggested by top-down chemical kinetics: heterogeneous nucleation and growth of C-S-H, lateral impingement of C-S-H regions, and further deceleration due to a decaying concentration of ions in solution. The proposed approach indicates a pathway for simulations to guide the design of architected nanopore structures, using both the solid and solution chemistry as levers to control the slow temporal development of microstructural texture and associated mechanical properties, such as autogenous stress and deformation.

(A4 oral) **Linear pore size dependence of water diffusion in nanoconfinement as assessed by noninvasive relaxometry method**

D Petit[1], H Chemmi[2], P Levitz[3], R Denoyel[4], A Galarneau[5] and J-Pierre Korb[2]

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We show that nuclear magnetic relaxation experiments at variable magnetic fields (NMRD) provide non-invasive means for probing the spatial dependence of liquid diffusion close to solid interfaces. These experiments performed on samples of cylindrical and spherical nanopore geometries demonstrate that average diffusion coefficient parallel to the interface is proportional to pore-radii in different dynamics regimes. A master curve method allows extracting gradients of diffusion coefficients at proximity of pore surfaces indicative of the efficiency of coupling between liquid layers. Due to their selectivity in frequency, NMRD experiments are able to differentiate the different water dynamical events induced by heterogeneous surfaces or composed dynamical processes. This analysis relevant in physical and biological confinements highlights the interplay between molecular and continuous description of fluid dynamics near interfaces.

[1] H. Chemmi, D. Petit, P.Levitz, R. Denoyel, A. Galarneau and J.-P. Korb, J. Phys. Chem. Lett. 2016, 7, 393-398

(A4 oral) **Effect of the curing temperature on the C-S-H composition and density in a Class G cement paste**

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The knowledge of the influence of the curing temperature on the microstructure of the cement paste is important for a better understanding of the behaviour of the cement sheath in oil-wells. Indeed, due to the geothermal gradient, the cement sheath along an oil-well is hydrated under different temperatures increasing with depth. This influences significantly the microstructure of the cement paste and decreases its mechanical properties. In the present work, the effect of hydration temperature, between 7°C and 90°C, on the microstructure of a hardened class G cement paste has been studied using a combination of various experimental techniques: X-Ray diffraction and Rietveld analysis, thermo-gravimetric analysis, mercury intrusion porosimetry, total porosity measurement. The analysis of the results of XRD-Rietveld and TGA experiments permitted the evaluation of molar C/S and H/S ratios for different temperatures, showing a decrease of these ratios with hydration temperature. The experimental results show an increase of the capillary porosity with hydration temperature, while the total porosity remains almost constant. The C-S-H density has been evaluated in an analysis combining the results of various experiments. The results show a densification of the C-S-H structure and a reduction of its internal porosity with increasing hydration temperature. This densification explains the observed increase of the capillary porosity and the resulted decrease of the cement paste mechanical properties for higher hydration temperatures.

(A5 invited) **3D image-based multiscale modeling of hierarchical porous electrodes: Mechanical strength and effective conductivity**

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The design of porous ceramic electrodes for Solid Oxide Fuel Cells presents the challenge of finding the best compromise between seemingly contradictory requirements: electrochemical performance and mechanical strength. Ceramic processing via ice-templating can be used to obtain anisotropic and hierarchical microstructures made of large oriented pores (few tens of microns) combined with nanopores left by partial sintering [1]. This kind of architecture advantageously provide solid matter in the direction of mechanic loading and ionic transport as well as large oriented channels in the direction of gas transport.

Modeling and simulations of mechanical and functional properties is required in order to tailor this system for high performing cathodes. The particulate and multiscale nature of the porous electrodes motivates the use of the discrete element method to model both their mechanical strength and effective conductivity. Discrete simulation have been performed on realistic microstructures generated from 3D images obtained by means of synchrotron X-ray nanoholotomography. The relevancy of the discrete approach is discussed by comparison with experimental results (mechanical strength) and fast fourier transform (FFT) simulations performed on Focus Ion Beam – Scanning Electron Microscopy tomography (effective conductivity).

[1] Lichtner, A. et al., J. Am. Ceram. Soc. 96, 2745–2753, 2013

(A5 oral) **Enhanced resilience of architected materials with hierarchical microstructures**

P Moretti and M Zaiser

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Materials with architected hierarchical microstructures are constituted by microstructural patterns that are repeated on multiple length scales in a self-similar fashion. Such hierarchical microstructures are extremely common in biological materials. Collagen for instance is well described in terms of a hierarchical modular structure, ranging from helical molecules, over microfibrils and fibers, to hierarchical fiber bundles, in which fibers are recursively grouped in larger super-structures. Other examples include the porous hierarchical structure of bone, the lamellar organization of seashells, and the cellular structure of wood. Such hierarchical order is conjectured to serve an essential purpose, that of ensuring load redistribution and damage containment. Hierarchical materials thus provide a promising route to the effective design of high-resilience architected materials.

We investigate the impact of hierarchical modular architectures on the resilience and the fracture mechanics of complex materials. We devise simple models of hierarchical fibrous microstructures and, by means of large-scale numerical simulations, we show how the inherent hierarchical stress redistribution leads to increased resilience, allowing hierarchical materials to outperform standard non-hierarchical fiber models. We show that, even under our simple assumptions, the hierarchical structure forces cracks to develop super-rough morphology and to undergo significant deflections, which limit their ability to propagate and significantly enhance fracture toughness.

(A5 oral) **Massively parallel FFT-based simulations to analyse the behaviour of architected SiC/SiC composite tubes from synchrotron X-ray tomography**

Y Chen[1], L Gélébart[2], F Ouaki[2], J Derouillat[2], C Sauder[2], C Chateau[3], P Aimedieu[3], M Bornert[3] and A King[4]

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Silicon carbide (SiC) is a material of interest for nuclear applications because of its stability at high temperature and under irradiation. In contrast with monolithic ceramics, architected SiC/SiC composites exhibit a quasi-ductile and reproducible behavior. Therefore, they are promising candidates for future fuel cladding tube applications.

The apparent ductility of SiC/SiC composites comes from the progressive development of a network of micro-cracks. Damage mechanisms have been deeply studied from biaxial tests on tubes together with surface observations and Digital Image Correlation [1]. To go further, in-situ tensile tests are performed on the X-ray tomography beamline Psiché (synchrotron SOLEIL) to characterize the 3D evolution of cracks (spatial distribution, orientation, …).

In order to discuss these results, numerical simulations are performed from the 3D images. Thanks to its massively parallel implementation, the FFT-based code AMITEX_FFTP [2] allows the simulation of large experimental unit-cells with high resolutions (1977x1977x555 in this case) to be realized. The non-classical use of FFT-based algorithm to simulate the response of a tube is discussed and the different pre-treatments (segmentation, alignment) performed on the 3D images to feed the numerical simulation are described. Finally, stress distributions are analyzed with respect to the microstructure and compared to the crack distributions to discuss the influence of the microstructure on damage mechanisms.

[1] F. Bernachy-Barbe, L. Gelebart, M. Bornert, J. Crepin, and C. Sauder. Characterization of SiC/SiC composites damage mechanisms using digital image correlation at the tow scale. Composites Part A: Applied Science and Manufacturing, 68(0):101 – 109, 2015.

[2] http://www.maisondelasimulation.fr/projects/amitex/html/index.html

(A5 oral) **Generation, compaction and strength of nanostructured silica aggregates using the discrete element method**

É Guesnet[1], D Jauffres[1], C Martin[1], R Dendievel[1] and B Yrieix[2]

[1]University of Grenoble Alpes, France, [2]EDF, France

Nanoporous materials are a natural choice for insulation materials. In particular, nanostructured silica powders are the preferred material for vacuum isolation panels (VIP) cores, with a thermal conductivity as low as 5 $mW.m^{-1}.K^{-1}$ versus 30 $mW.m^{-1}.K^{-1}$ for standard materials. The large amount of nanoporosity of these materials greatly decreases the thermal conductivity, however it also leads to poor mechanical properties.

Our goal is to model and simulate the mechanical behaviour of various types of nanostructured porous silica considered for PIV applications (fumed silica, precipitated silica and aerogel grains), to better comprehend the origin of their brittleness and to optimize the microstructure for the best strength / low thermal conductivity compromise. Low thermal conductivity is related to the nanoscale characteristics of the porosity while the strength originates from aggregate bonding at a larger scale.

The modelling approach chosen, the discrete element method (DEM), is particularly well-suited to model damage and fracture behaviour of porous materials with granular characteristics (Pizette, P. et al. J. Eur. Ceram. Soc. 33, 975–984 (2013)). Nanosilica aggregates are numerically generated and isostatically compacted to obtain numerical samples with realistic microstructures. These samples are characterized for strength via numerical tensile tests with appropriate microscopic strength criterion.

(A5 oral) **Assessing the fracture strength of geological and related materials via an atomistically based J-integral**

R Jones and L Criscenti

Sandia, USA

Predicting fracture in low-permeability geomaterials is a critical yet unsolved problem crucial to assessing shale at carbon sequestration sites, and controlling fracturing for hydrocarbon extraction. Experiments indicate that chemical reactions at fluid-geomaterial interfaces play a major role in subcritical crack growth by weakening the material. Engineering the subsurface fracture environment, however, has been hindered by a lack of understanding of the mechanisms relating chemical environment to mechanical outcome, and a lack of capability directly linking atomistic insight to macroscale observables.

We have developed a fundamental atomic-level understanding of the chemical-mechanical mechanisms that control subcritical cracks through coarse-graining data from reactive molecular simulations. Previous studies of fracture at the atomic level have typically been limited to quantifying either the system-level stress or energy at which fracture propagation occurs. As such, these curves are neither characteristic of nor insightful regarding fracture at the crack tip. In contrast, configurational forces, such as the J-integral, are specific to the crack in that they measure the energy available to move the crack and truly quantify fracture resistance. By development of field estimators consistent with the continuum conservation properties we are able to connect the data produced by atomistic simulation to the continuum-level theory of fracture mechanics and thus inform engineering decisions. In order to trust this connection we have performed theoretical consistency tests and validation with experimental data. Although we have targeted geomaterials, this capability can have direct impact on other unsolved technological problems such as predicting the corrosion and embrittlement of metals and ceramics.

(A6 invited) **Role of mesoscale structure in the mechanical behaviour of self-standing thin clay films**

M Vandamme[1], B Carrier[1], R Pellenq[2], M Bornert[1], E Ferrage[3], F Hubert[3] and H Van Damme[2]

[1]Ecole des Ponts ParisTech, France, [2]UMI 3466 CNRS-MIT, France, [3]Université de Poitiers / CNRS, France

This study focuses on the mechanical behaviour of self-standing montmorillonite clay films with a thickness of a few dozen micrometers. In particular, we look at their elastic stiffness and their propensity to creep. Here, we characterize the dependence of those properties on relative humidity (or water content) and on the interlayer cation.

The films are manufactured by evaporation of a clay suspension on a substrate, from which they are peeled off. The elastic and creep properties are measured by performing tensile experiments on the films, in a temperature- and humidity-controlled environment. During those experiments, strains are measured by digital image correlation, which is a contact-free technique.

We discuss our experimental results by comparing them with the mechanical properties of the nanometer-thick clay layers constituting the films, which we obtained by molecular simulations. We observe significant qualitative differences between the elastic and creep properties of the clay layers and those of the clay films, in particular in how those properties depend on water content and on the interlayer cation. From this discrepancy, we infer that the mechanical behaviour of the films is significantly impacted by the structure of the films at a scale greater than that of the clay layer, i.e., by a mesoscale structure.

(A6 oral) **Small-angle scattering analysis of empty or loaded hierarchical porous materials**

C Gommes

University of Liege, Belgium

Small-angle scattering (SAXS or SANS) is one of the few experimental methods available for the nanometer-scale study of physicochemical phenomena inside porous solids. Its potential, however, is often limited by the lack data analysis methods to convert scattering data into real-space structural information. This is notably the case for most porous materials of practical interest, which exhibit a hierarchical structure with micro, meso, and macropores, with often a secondary material confined in the pores, such as in supported catalysts, as well as fuel-cell and battery materials.

Here, we discuss a general SAXS data analysis methodology for this type of material. Assuming that each structural level is statistically independent from the others and has a distinct characteristic length scale, compact mathematical expressions are derived for the scattering of the entire hierarchical structure [1]. The method is illustrated with the SAXS analysis of SBA-15 micro- and meso-porous silica loaded with copper nitrate, as well as to supported catalysts obtained after calcining that material. The SAXS analysis shows that the nitrate permeates both the micro and mesopores, while the metallic copper obtained after calcination is found only in the mesopores. Moreover, the spatial distribution of the metal depends on the specifics of the calcination, as confirmed by electron tomography [2]

The general methodology will be of interest to anyone interested in the quantitative analysis of small-angle scattering data from empty or loaded porous solids, and from any type of hierarchical material.

[1] J.Phys.Chem.C, in press
[2] Angew.Chem.Int.Ed. 54 (2015) 11804

(A6 oral) **Combined experimental-modeling approach towards better predictions of fruit tissue dehydration**

K Prawiranto[1], T Defraeye[2], D Derome[1] and J Carmeliet[2]

[1]Empa, Switzerland, [2]ETH Zürich, Switzerland

Fruit is a soft cellular material that undergoes microstructural changes during dehydration, including large deformations, cell membrane breakage and cell wall collapse. These changes have a significant impact on its macroscopic properties, e.g. moisture permeability, during dehydration. Although this permeability is critical for continuum modelling of fruit dehydration, its variation during drying due to microstructural changes is not known. Such information is however imperative in hygrothermal finite-element simulations for accurate predictions of drying kinetics and internal moisture content distributions. This study aims to determine the variation of the effective moisture permeability of apple tissue during dehydration, by taking into account the impact of microstructural changes. To this end, an upscaling methodology, utilizing cellular scale data to provide continuum properties, is presented.

X-ray tomography is used to unveil the apple tissue microstructure (cell size, porosity and tortuosity) at different stages of dehydration. The information is transferred to a microscale model to determine the effective moisture conductivity in the cellular material. Simulations are run for different cellular structures according to corresponding dehydration stages. The calculated effective moisture permeabilities show a strong moisture content dependency. Using this upscaled moisture permeability, the drying characteristics of apple slices are quantified using the hygrothermal continuum model. The results are validated against data from drying experiments in a climatic-controlled room and from neutron tomography. This multiscale approach is capable to better predict the drying kinetics and moisture distribution of the fruit, including in extreme dehydration stages.

(A6 oral) **Modeling the transport of water and ions tracers in a micrometric sample of clay**

P Bacle[1], J-F Dufrêche[2], B Rotenberg[1], I C Bourg[3] and V Marry[1]

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Numerous experimental and theoretical studies have focused on predicting the performances of clay minerals as barrier materials in the containment of high-level radioative waste by evaluating the diffusion of mobile species in compacted, water-saturated Na-bentonites. One difficulty arises from the complex, multi-porosity structure of clay materials.

We present a simple model which enables us to investigate the transport of water and ionic (Na^+, Cl^-) tracers in a micrometric sample of clay. Here, the clay particles are modeled by cylindrical platelets the dimensions of which are calculated according to the density of clay. The cylinders can overlap each other which allows us to reach high densities and thus investigate the diffusion in highly compacted porous media. We use Brownian Dynamics to describe the diffusion of the tracers in the sample. Our porous medium consists of two environments (the platelets and the interparticle pores) and the diffusion coefficient of the tracer varies with regard to its location within the simulation box: The diffusion outside the platelet is the same as in the bulk solution but the diffusion inside the platelets is slowed by the confinement and depends on the charge of the tracer. The concentrations and the diffusion coefficients in the two environments are used as simulation parameters and are calculated based on experimental values and /or determined from molecular dynamics simulations. We evaluated the global diffusion coefficients of the tracers for various densities and salinities from their trajectories and compared the simulations results with experimental data from tracer diffusion experiments.

(P1.01) **Assessing the fracture strength of geological and related materials via an atomistically based J-integral**

R Jones and L Criscenti

Sandia, USA

Predicting fracture in low-permeability geomaterials is a critical yet unsolved problem crucial to assessing shale at carbon sequestration sites, and controlling fracturing for hydrocarbon extraction. Experiments indicate that chemical reactions at fluid-geomaterial interfaces play a major role in subcritical crack growth by weakening the material. Engineering the subsurface fracture environment, however, has been hindered by a lack of understanding of the mechanisms relating chemical environment to mechanical outcome, and a lack of capability directly linking atomistic insight to macroscale observables.

We have developed a fundamental atomic-level understanding of the chemical-mechanical mechanisms that control subcritical cracks through coarse-graining data from reactive molecular simulations. Previous studies of fracture at the atomic level have typically been limited to quantifying either the system-level stress or energy at which fracture propagation occurs. As such, these curves are neither characteristic of nor insightful regarding fracture at the crack tip. In contrast, configurational forces, such as the J-integral, are specific to the crack in that they measure the energy available to move the crack and truly quantify fracture resistance. By development of field estimators consistent with the continuum conservation properties we are able to connect the data produced by atomistic simulation to the continuum-level theory of fracture mechanics and thus inform engineering decisions. In order to trust this connection we have performed theoretical consistency tests and validation with experimental data. Although we have targeted geomaterials, this capability can have direct impact on other unsolved technological problems such as predicting the corrosion and embrittlement of metals and ceramics.

(P1.02) **Influence of the yield stress on the evolution of a bubble population in a viscoplastic fluid: Consequences on the macroscopic swelling of bitumen drums**

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The context of this study is to predict the swelling of bitumen drums in which radioactive salts are mixed (60% wt of bitumen and 40% wt of salts). Radioactivity generates uniform volume production of hydrogen by radiolysis of bitumen chains and leads to bubble nuceation and growth. Since the production rate of gas occurs on very large time scales (more than a hundred years), one needs to set up models to predict the material swelling. It has been shown that bitumen is a yield stress fluid. The present work therefore proposes to study the influence of the yield stress and the production rate of gas on the evolution kinetics of a bubble population. Usually, in a non-yield stress fluid and without gas creation, a supersaturation of gas leads to a scenario of germination, bubble growth and Ostwald ripening (growth of large bubbles at the expense of the small ones). Over long times, a self-similar distribution of large bubbles is selected, independent of the initial distribution of nuclei. In this work, a new model for bubble growth in an infinite viscoplastic material is introduced. Then it is shown that there exist conditions for which the production rate of gas competes with the kinetics of ripening and where the yield stress induces hysteresis and pulsing phenomena on the kinetics of bubbles distribution. The effect of the yield stress and the initial distribution of nuclei on the final population and on the macroscopic swelling of the fluid is discussed.

(P1.03) **Modelling the support effect on the flux through an asymmetric oxygen transport gas separation membranes**

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Oxygen Transport Membranes (OTM) display a new technology for energy-efficient oxygen generation which can be used in low-pollutant power plants and oxygen generators or membrane reactors in the chemical industry and health care. Low ionic resistance of the membrane and high mechanical stability typically demands the usage of an asymmetric design comprising a thin functional membrane and a thicker porous support. The overall membrane performance is strongly affected by the microstructure of this porous structural layer. The effect of the support on the flux performance has been thus studied applying the Binary Friction Model (BFM, including binary and Knudsen diffusion and viscous flow) for the support together with a modified Wagner equation for the dense membrane. The parameters describing the tape-cast porous medium were obtained by numerical diffusion and flow simulations based on micro computed tomography (µCT) data. Using different flow conditions (3-end, 4-end) and oxygen as feed gas, the effect of the support thickness, pore diameter, position (either on the feed or permeate side) of the support on the flux were investigated. Knudsen diffusion was found to dominate the transport process for small pore sizes (~2µm) in particular for the 3-end mode with the support on the permeate side being most pore size sensitive, whereas for the other configurations the viscous flow was of higher significance. For typical membrane assembly geometry with a membrane thickness of 20 µm and a support thickness of 0.9 mm, the flux became membrane limited starting from a pore size of approx. 5 µm.

(P1.04) **Wind load effect on silkworm silk fiber web structure**

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Optimized by nature, silk exhibits remarkable mechanical strength, toughness and robustness to fulfil specific functions. Silk's impressive properties originate from its hierarchical organization making it an inspiration for upscaling molecular properties to the macroscale. Silk is a protein which sequence dictates protein folding and consequently its macroscale mechanical properties. Silk's stiffness arises from the crystalline region and its extensibility from the hidden length within the semi-amorphous region. As for cocoons, they have a complex three-dimensional multi-layered structure composed of a porous matrix reinforced of randomly oriented fibres. They are designed to withstand wind load. However, this study investigates how a single-layer silk architecture deflects and fails under wind load.

Here, experiments in the wind tunnel and simulations were carried out to investigate wind load effect on a cocoon silk web. The webs are spun by silkworms and subjected to an increasing wind load until failure. The models created are inspired from microscopic scans and SEM of actual webs. Before failure, webs can deflect up to 11.4 mm at 38.9 m/s wind speed. Simulation results have shown the crucial role of fibre organization and web porosity in the robustness of the structure.

Understanding the mechanics across scales between fibres and the complex architecture of the web could contribute to material and structural optimization for bio-inspired composite material design. In particular, silk web-inspired designs could lead to high-performance, resilient and lightweight fibre-based materials.

(P1.05) **Grain growth in porous oxides**

A El-Azab[1] and K Ahmed[2]

[1]School of Materials Engineering, USA, [2]Purdue University, USA

We present a phase field model for investigating grain growth in porous oxides with applications to UO_2 and CeO_2. The model takes into account the interactions between pores and grain boundaries, as well as the pore mobility. Using a formal asymptotic analysis, the phase field model was matched to its sharp-interface counterpart and all model parameters were uniquely determined. Therefore, the model is able to obtain accurate growth rates that can be compared with experiments. The model was used to reveal various growth regimes in porous oxides, boundary-controlled versus pore-controlled growth kinetics. The model results showed that the pore breakaway phenomenon can only be observed in 3D simulations. The important features of the model and results will be presented.

(P1.06) **Synthesis of geopolymer foams**

P Svetlana and P Arnaud

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The aim of this work is to synthesis inorganic foams from geopolymer cements for the decontamination of liquid radioactive waste. Geopolymers are a class of mesoporous binders obtained by alkali activation of an aluminosilicate source (here the matakaolin) at room temperature. The use of the intrinsic mesoporosity and the high specific surface area of the geopolymer will allow to graft and trap selectively the radionuclides of interest and the creation of connected macroporosity will facilitate the transport of contaminated fluid. To generate a foam, several parameters have to be controlled such as:

- the source term namely the production rate gas,
- the nature and content of surfactants which govern the surface tension between the gas and the paste and avoid the coalescence,
- the rheological behaviour which continuously evolves over time and governs the convection process.

In the present study, a sodium geopolymer is studied and hydrogen peroxide is used as blowing agent. The results show that it is possible to obtain a low density material and to control the bubbles size distribution according to the concentration of surfactants and the formulation parameters of the geopolymer. Moreover, some 3D observations by X-ray tomography show that the macroporosity is completely connected which will facilitate the transport of fluid.

In parallel, the modelling of the formation of these inorganic foams by the description of all the physical phenomena such as the source term, the nucleation and growth process, the rheological behaviour and the swelling is in progress.

(P1.07) **Separation of pore cluster and defect influences on the failure behaviour of Macro-Porous Ceramics**

P D Krummrich and T Hochrainer

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Macro-porous ceramics are characterized by distributions of macro-pores and matrix defects. Correlations between pore distribution characteristics and the failure behaviour may be investigated by mostly two dimensional Finite-Element simulations of so called representative volume elements (RVE).

RVEs are typically subjected to periodic boundary conditions. Moreover the matrix is commonly simplified as homogenous. The significance of such simplified simulations needs to be validated, especially if the matrix failure is potentially dominated by matrix defects.

To validate the matrix material model we present a quasi-periodic specimen design, which we use to differentiate between pore and matrix defect influences. A quasi-periodic specimen is designed such that the internal stress state closely resembles the stress state in the conforming periodic RVE. The differentiation is based on a comparison between simulated and experimentally observed crack paths inside corresponding volume elements.

We validate the concept of the quasi-periodic specimen design with Polymethylmethacrylat specimens using the photoelastic effect. The experimentally observed crack paths are nearly the same as in a corresponding RVE simulated with a homogeneous matrix and a principal stress based failure criterion. In the current work we transfer the concept to macro-porous Aluminumoxid. The defect distribution inside the matrix is tailored by the sintering process. We found bounds regarding the size distribution of matrix defects in relation to the average macro-pore size. The mechanical failure is clearly dominated by the macro-pore distribution under these bounds.

(P1.08) **Acoustic properties of ceramic micro-scaffolds: FEM analysis and experiments**

A Kruisova[1], P Sedlak[1], M Sevcik[1], H Seiner[1], M Landa[1], B Roman-Manso[2], P Miranzo[2] and M Belmonte[2]

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Robocasting is an additive manufacturing methods that enables fabrication of micro-scaffolds consisting of fully dense ceramic rods with prescribed periodical spatial arrangements. Such scaffolds exhibit unique acoustic properties, for example strong anisotropic focusing of acoustic energy, mixing of wave-propagation modes, and very low internal friction. Most importantly, the periodicity of the internal architecture of the scaffolds leads to a frequency band structure for propagation of acoustic waves.

In this contribution, six different periodic geometries of the scaffold will be studied from the point of view of their frequency band structure. As shown by finite elements calculations (FEM), the band structure depend strongly on the symmetry class of the internal architecture of the scaffold, as well as on the geometry parameters such as thickness of the rods or the spacing's between them.

The results of the FEM calculations will be compared with the experimental spectrograms obtained on real robocast silicon carbide micro-scaffolds. It will be shown that for simple geometries (rectangular with a tetragonal arrangement of rods) the FEM calculation predicts quite well the locations of the lowest frequency band-gaps, while for more complex architectures, such as hexagonal or rhomboidal, the band structure becomes very involved. For these complex architectures, the calculated band structure reveals several interesting metamaterial-like features, which indicates that these scaffolds may find interesting applications in acoustic lensing or acoustic energy redistribution.

(P1.09) **From 3D images to 3D printed optimized materials**

S Chupin and D Rochais

CEA, France

Since a few years, a small revolution is happening in material science through the development of experimental techniques leading to get the 3D representation of significant volume of material at a representative scale (TEM, FIB/SEM, X-Ray micro-tomography). Thus, using more and more powerful image processing techniques, new microstructural analysis approaches arise to study materials from nanometers to millimeters scales. Moreover, recent computer abilities (especially high performance computing solutions) allow to achieve numerical experiences to estimate some physical properties of materials through the use of their 3D numerical description. Nevertheless, these computations can only be done if the properties of each component of the material are known at the appropriate scale.

Beyond the estimation of properties of a given material, these simulations enable the development of optimized materials. In fact, the 3D microstructure can be numerically transformed or can be entirely designed by computer. Also, in numerical simulations, the base component properties can be easily changed. Then, according to thermal and/or mechanical specifications, an optimized material can be designed by changing either the microstructure and/or the base component properties.

The last thing is to make and test these optimized materials... It's in this context that additive manufacturing (or 3D printing) is used. This process leads to build optimized complex structures than cannot be made by conventional processes. Also the same process can provide elementary samples to estimate local properties simply at the good scale. Then, computational results and real thermal or mechanical experiments can be compared.

(P 1.10) **Mechanical behavior of silica aerogel using Molecular Dynamics simulations: the first modelling step for a multi-scale approach**

W Gonçalves[1], P Chantrenne[1], J Morthomas[1], M Perez[1], J Amodeo[1], G Foray[1] and C Martin[2]

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Novel optimized materials offering very high thermal resistance and minimal thickness are needed for the conservation of energy in the building and transportation sectors. Silica aerogel super insulation materials could match these strict standards with their exceptionally low thermal conductivity (< 20 mW/m.K). Their tortuous nano-porous structure provides the desired thermal properties but is also responsible for their poor mechanical properties. These granular-like materials present a multi-scale structure originating from the sol-gel process and their ambiant air drying. In this investigation, we show how these mechanical properties can be modelled using a multi-scale approach.

The purpose of this study consists in using Molecular Dynamics (MD) simulations to predict the mechanical behavior and contact laws between two porous nanoparticles of silica aerogel. The selected interatomic potential (A. Carré et al., J. of Chem. Phys. 127,114512 (2007)) is a truncated and screened version of the widely used BKS potential. A previous study has already demonstrated the capability of this truncated potential to reproduce amorphous silica surface properties. First, mechanical tests on silica aerogel structures are performed using periodic boundary conditions. The influence of strain rate is discussed and an appropriate representative elementary volume is inferred from the simulations. Thus, porous nanoparticles are cut out of the original structure and the interparticle behaviour is investigated during compaction. Deformation mechanisms are investigated and contact laws are implemented in a Discrete Element Method (DEM) code required to model aggregates at the scale of the experiment.

Symposium B

(B1+E7 oral) **Revealing the mechanism of Z phase-formation in 12% Cr ferritic-martensitic steels**

D Urban, M Mrovec and C Elsässer

Fraunhofer IWM, Germany

The challenge of raising the steam inlet temperature of fossil-fired power plants calls for ferritic-martensitic creep-resistant steels with a Cr content of 11-12% in order to achieve sufficient corrosion and oxidation resistance. However, it has been found that in steels strengthened by fine (V,Nb)N particles, these precipitates transform during long-term service into coarse, thermodynamically more stable Z-phase particles, CrMN (M=V,Nb,Ta), that deteriorate the steels' mechanical behavior.

We present extensive atomistic simulations, using density function theory, that help to understand the essential mechanisms underlying the formation of the detrimental Z-phases. Our results reveal that the Z-phase transformation proceeds via diffusion of Cr atoms into the MN particles and their subsequent clustering in a layered arrangement of the Z-phase. We systematically scan the configuration space of various predecessor structures by varying their morphology, stoichiometry and point defect concentration. Our results support experimental efforts to control the precipitation of the Z-phase through appropriate microstructural engineering.

(B1+E7 oral) **Mesoscale model of stacked organic light emitting diodes**

A Walker[1], I Thompson[1], W Wenzel[2], F Szymalla[2] and V Meded[2]

[1]University of Bath, UK, [2]Karlsruher Institute of Technology, Germany

A 3-Dimensional mesoscale simulation has been undertaken of the electrical and optical characteristics of a stacked organic light emitting diode, OLED. Our Kinetic Monte Carlo approach adapted from organic solar cell simulations adds considerable capability to well established techniques of OLED simulation by allowing for interactions between the particle species, here electrons, holes, singlet and triplet excitons. We show that the materials composition and layer widths influence the recombination zone location and can significantly improve OLED output if materials and layer widths are chosen appropriately. If the recombination zone is narrowed, there is an improvement in the singlet generation yield via triplet-triplet reactions that can cause as much as an order of magnitude increase in the luminous efficiency. We examine the effects of changes caused by altering layer widths on the exciton formation efficiency and of outcoupling of light from the device which can compete. Both these effects are very sensitive to materials composition and geometry.

(B1+E7 oral) **Gathering materials properties from literature for the design of new materials**

L Kunz[1], B Ziebarth[1], L Weber[2] and T Eckl[1]

[1]Robert Bosch GmbH, Germany, [2]OntoChem GmbH, Germany

The design of new materials can strongly benefit from material properties which have been published in literature within the last century. But unlike crystallographic data most of the materials data is not collected in a structured way, which impedes the systematic analysis to identify unknown correlations.

A manual extraction of material properties however cannot be achieved in a reasonable time. Therefore we developed first materials ontologies and used the software OCMiner® from OntoChem to efficiently extract material properties from publications, books and patents. This data has been combined with existing crystallographic databases e.g. Inorganic Crystal Structure Database (ICSD) and crystallographic open database (COD) as well as ab-initio databases like Materials Project and the Open Quantum Materials Database (OQMD) into a materials data warehouse which forms the basis for the discovery of new materials.

We will present first extraction and analysis results and address open topics like microstructure ontologies. We hope this will inspire subsequent discussions on a community effort to create a common ontology for materials informatics.

(B2 invited) **Harnessing electronic structure for engineering alloy design through big data**

K Rajan

University at Buffalo-the State University of New York, USA

This presentation provides an overview of how by harnessing the tools of "BigData" analytics, one can map the high dimensional nature of the systematics of electronic structure data fingerprints into the property space of engineering alloys. Examples are given where by using the computational framework of manifold learning, one can guide first principle calculations that identify the influence of specific elements on phase stability, crystal structure, elastic properties and beyond to engineering scale performance including environmental stability and high temperature mechanical properties. The predictions of the methodology are shown to be consistent with reported experimental and theoretical studies. The informatics based methodology presented in this study can be generalized to a framework for data analysis and knowledge discovery that can be applied to many materials systems and recreated for different engineering design objectives.

(B2 oral) **High-Throughput approach for the discovery of novel hardmagnetic phases**

G Krugel, W Körner, M Senn, D Urban and C Elsässer

Fraunhofer IWM, Germany

High-performance permanent magnets are key materials for environmentally friendly technologies and indispensable for wind turbines and electro mobility. A high-throughput approach is carried through to identify novel hardmagnetic materials with a reduced amount of rare-earth elements. The tight-binding–linear-muffin-tin–atomic-sphere-approximation is applied as a fast DFT method.

The computational high-throughput screening approach [1] is extended by approximate evaluations of the anisotropy coefficient K_1, the anisotropy field H_a and an estimation of the energy product (BH). The implemented calculation of K_1 is fast since it is based on the crystal field parameters and avoids expensive total-energy calculations. Examples will be given to demonstrate the application of statistical methods for the evaluation of the resulting data.

[1] N. Drebov et al, New J. of Phys. 15, 125023 (2013)

(B2 oral) **Interstitial solution enthalpies derived from first-principles: Knowledge discovery using high-throughput databases**

U Aydin, T Hickel, J Janssen and J Neugebauer

Max-Planck-Institut für Eisenforschung GmbH, Germany

Interstitial elements play a decisive role for the performance of transition metals. Carbon, for example, is important for microstructure formation; hydrogen is known to yield embrittlement phenomena; boron can support the stabilization of grain boundaries, while oxygen yields their internal oxidation. Furthermore, the strain imposed by interstitial elements is often used to trigger magnetic or structural properties of compounds. The computational design of innovative materials therefore requires the reliable prediction of interstitial concentrations.

We have extended and applied our python-based high-throughput workbench in order to reveal the underlying physical mechanisms that determine interstitial solution enthalpies in transition metals. A careful first principle analysis has started with hydrogen to identify possible chemical and mechanical descriptors that determine the solubility. The study was in a second step extended to first-principles calculations of hundreds of solute-solvent combinations along with the determination of the physical properties of the host materials. In order to analyse the data, complex simulation protocols based on Pearson correlation coefficients, factor analysis, and singular value decomposition have been implemented into our workbench. As a result we have discovered a previously unknown formula containing only a few descriptors, which captures the solution process for all solute-solvent combinations with high accuracy. It allows one to predict interstitial concentrations solely from the knowledge of a couple of host-material properties such as bulk modulus and bandstructure parameters. The formula is used to reveal and design the solubility of interstitials in (multi-component) materials that were not incorporated in the high-throughput study.

(B2 oral) **Three-parameter crystal-structure prediction for sp-d valent compounds**

T Hammerschmidt, A Bialon and R Drautz

ICAMS / Ruhr-Universität Bochum, Germany

The prediction of the crystal structure of a material from only its chemical composition is one of the key challenges in materials design. We use a cluster analysis of experimentally observed crystal structures and derive structure maps that are systematically optimised to reach high predictive power. In particular, we present a three-dimensional structure map for compounds that contain sp-block elements and transition metals in arbitrary composition. The structure map predicts the correct crystal structure with a probability of 86% and has a confidence of 98% that the correct crystal structure is among three predicted crystal structures. The three parameters that span the structure map are physically intuitive functions of the number of valence electrons, the atomic volume and the electro-negativity of the constituent elements. We test the structure map against standard density-functional theory calculations for 1:1 sp-d-valent compounds and demonstrate that our three-parameter model has comparable predictive power. We show that the identified parameters are valid for off-stoichiometric compounds and that they separate binary and ternary crystal-structure prototypes.

(B3 invited) **First-principles materials exploration of piezoelectrics**

T Oguchi and H Momida

Osaka University, Japan

Piezoelectrics are widely used nowadays in various ways such as sensors, actuators, and filters in modern electronic devices. In recent applications, one of the most frequently utilized piezoelectrics is metal oxide ceramics such as Pb-Zr-Ti-O, which shows a high piezoelectric constant of ~ 410 pC/N at temperatures up to ~ 250°C, and there are growing demands for exploring novel materials usable in higher-temperature environments for automobile applications. AlN is highly expected to be a candidate for such high-temperature applications due to its high Curie temperature of ~ 1150°C, and significant enhancement of piezoelectricity by alloying with Sc has been recently found experimentally, attracting much interest in technological as well as scientific fields. In this context, we computationally investigate microscopic mechanisms of the piezoelectricity enhancement of $Sc_xAl_{1-x}N$ materials by means of first-principles calculations, providing guiding principles to design highly piezoelectric materials. AlN has the wurtzite crystal structure, and several $Sc_xAl_{1-x}N$ model structures are adopted by substituting Al with Sc for wide composition range of x=0–1. Calculated results clearly demonstrate that the piezoelectric responses of $Sc_xAl_{1-x}N$ increase with increasing Sc concentration (x), as reported by the experiments and calculations. Calculated piezoelectric constants are scattered especially in high x values depending on different spatial distributions of Sc atoms in the models. A general trend in piezoelectricity versus structure parameters on the basis of our theoretical investigations for the materials with the wurtzite structure leads to further exploration of promising piezoelectric materials.

(B3 oral) **Synthetic screening of electrolytes for Li-Air batteries**

R Jones, F Gittleson, D Ward, M Foster and M Anstey

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There is increasing interest in designing and manufacturing high-performance batteries for a wide variety of applications; however, finding the best electro-chemical system and configuration is a chal- lenging task given all the possibilities. In particular, choosing an electrolyte optimal for a given battery configuration and chemistry is a daunting and crucial task in and of itself. We propose a computational approach to electrolyte screening and selection for a Li-air battery. Li-air batteries are particularly attractive for mobile and transportation applications given their high theoretical volumetric and gravimetric energy densities, which in part is due to using environmental oxygen. Through a combination of techniques, starting with ab initio calculations to provide fundamental parameters, to molecular dynamics which, in turn, provides transport coefficients to a full-scale model battery, we can predict battery performance. Predictions using these techniques spanning many spatio-temporal scales are compared with a limited set of cyclic voltammetry experiments for validation before applying the process to a wide range of solvent, salt and other permutations to select the best candidates for intensive development. The concept of computational screening for battery development is not novel, e.g. Ceder et al, but here we focus on identifying ideal electrolytes for Li-air batteries where the diffusion of dissolved Li ions and molecular oxygen have been identified as power performance metrics.

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

(B3 oral) **Tight-binding quantum chemical molecular dynamics simulation on chemical reaction between organic carbonate and li anode in li-air battery**

K Watanabe, Y Ootani, Y Higuchi, T Nishimatsu, N Ozawa and M Kubo

Tohoku University, Japan

Organic carbonate such as ethylene carbonate (EC) is used as electrolyte for Li-air battery. Because the quality of solid electrolyte interface (SEI) generated by the chemical reactions between electrolyte and Li anode influences on Li^+ conductivity, it is necessary to reveal the generation mechanism of SEI for the high Li^+ conductivity. We investigated the generation mechanism of SEI on the Li anode by analysing the chemical reaction dynamics of EC with a Li surface via our tight-binding quantum chemical molecular dynamics simulator. To reveal chemical reactions between an EC and a Li anode surface, one EC was set on Li(100). We observed generation of two O-Li bonds between the EC and Li(100), and adsorption of the EC on Li(100). Then, the two C-O bonds of the EC were cleaved and the EC was decomposed into CO_3 and C_2H_4. We continued to add EC one by one on Li(100). After the 5^{th} EC was added, we observed lift of Li atom interacting with two or three O atoms of CO_3. The Li atom reached the surface and interacted with the O atom of the added EC. Then, the added EC was decomposed. The SEI was grown through these chemical reactions. After the 24^{th} EC was decomposed, the chemical composition of the SEI was $Li_{1.67}CO_3$. This means that the SEI contains Li defects. We suggest that the existence of Li defects enhances the Li diffusion in SEI. We successfully revealed the chemical reaction dynamics and the generation of SEI containing Li defects.

(B3 oral) **Investigating the relation of molecular conductance and structure for thousands of junction geometries**

H Vazquez

Inst. of Physics, Academy Sciences of the Czech Republic, Czech Republic

Single molecule circuits, where an electrical current is passed across a molecule placed between two electrodes, are ideal systems for studying a range of quantum phenomena. Recently the combination of theory and experiment has highlighted the important role that quantum interference can play at these junctions. There have been several examples of destructive interference where conductance goes to zero [1,2]. Similarly, we recently studied the conductance superposition law in molecular circuits and demonstrated constructive quantum interference effects [3]. We showed that molecules with two branches bound in parallel to the electrodes can exhibit more than twice the conductance of the single backbone counterparts.

Here we apply an approximate method to calculate molecular conductance and combine it with Molecular Dynamics (MD) simulations of the junction to analyze the evolution of junction structure and conductance. The affordable computational cost of this approximation enables the calculation of thousands of junction structures. In our study we analyze the junction structural parameters (eg. bond lengths, dihedral angles) and discuss their effect on conductance. We focus on the structure of the double backbone molecule and its relation to the degree of constructive quantum interference.

[1] D. Fracasso, H. Valkenier, J.C. Hummelen, G.C. Solomon and R.C. Chiechi, JACS 133 9556 (2011)
[2] C.M. Guedon, H. Valkenier, T. Markussen, K.S. Thygesen, J.C. Hummelen and S.J. van der Molen, Nature Nanotechnol. 7 305 (2012)
[3] H. Vazquez, R. Skouta, S. Schneebeli, M. Kamenetska, R.Breslow, L. Venkataraman and M.S. Hybertsen, Nature Nanotechnol. 7 663 (2012)

(B3 oral) **Atomic-green's-function approach to phonon scattering by extended defects in silicon**

T Wang[1], J C Montana[2], N Mingo[2] and G K H Madsen[1]

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Predicting the thermal conductivity of semi-conductor devices is an inherent multi-scale problem. It requires the quantification of phonon scattering strength caused by various types of defects e.g. vacancies, interfaces and dislocations, inside the industrial materials. For the defects that strongly perturb the neighbor environment, the Born approximation of the associated perturbation to the system will fail. The Atomic-Green's-Function approach has been demonstrated to be an efficient way to evaluate such phonon scattering events.[1]

For a one-dimensional line defect, we demonstrate a formalism, where the three-dimensional Brillouin Zone (BZ) is divided into parallel two-dimensional planes perpendicular to the defect line direction. A triangulation mesh is adopted to discretize each of the two-dimensional BZ planes. This treatment allows us to split the three-dimensional domain into independent two-dimensional domains and obtain Green's function in defected super-cell. By summing all the results of the planar sub-domains, the T-matrix and scattering cross section are obtained.

We will illustrate this strategy by setting up an atomic model of a quadrupolar arrangement of edge dislocations in silicon using linear elastisity theory. The frequency frequency dependence of the scattering rate is calculated and it is discussed how this form the basis of a all-scale calculation of the thermal conductivity.

[1] Katcho et. al. Phys. Rev. B 90, 094117 (2014)

(B4 invited) **Optimization of nanostructured materials for thermoelectric and electrothermal applications**

A Shakouri[1], J-H Bahk[2], Y Koh[1], A M Shahat[1], M Zebarjadi[3] and J Zide[4]

[1]Purdue University, USA, [2]University of Cincinnati, USA, [3]Rutgers University, USA, [4]University of Delaware, USA

More than 90 % of primary energy is first converted to heat, but only 12 % is transformed to end-use applications. Currently, there are no commercially available large-scale waste heat recovery systems. Thermoelectric is a solid-state device that can directly convert heat to electricity and vice versa. The improvement in the efficiency of thermoelectric energy conversion has been slow because all the material properties comprising ZT are mutually coupled, and it is extremely difficult to enhance one property without affecting another. Nanostructuring with embedded nanoparticles has been proposed as a mean to improve electrical conductivity with modulation doping, increase the Seebeck coefficient by hot electron filtering and to reduce thermal conductivity by scattering mid-long wavelength phonons. Systematic optimization of embedded rare-earth semi-metallic nanoparticles (ErAs, TbAs, …) in III-V semiconductors will be described. While ZT has been improved by a factor of two to about 1.5, challenges in predicting electronic bandstructure near nanoparticles and co-optimization of the electrical and thermal properties will be highlighted. Recent studies of quasi-ballistic heat flow using time-domain thermoreflectance demonstrate the importance of fractal Lévy random flights for phonons at a length scale of couple of microns and a time scale of 0.1-10ns. Implications in engineering nanoscale thermal transport will be described. This has also implications in the optimization of materials and interfaces for high power electronic devices.

(B4 oral) **Ab-initio modeling of thermal transport beyond the single crystal: effects of size, defects, dimensionality, and soft modes.**

N Mingo[1], B Vermeersch[1], A Van Roekeghem[1], J Carrete[1], A Katre[1], N Protik[2], D Broido[2], L Lindsay[3], N Katcho[4] and J Gallego[5]

[1]CEA-Grenoble, France, [2]Boston College, USA, [3]Oak Ridge National Laboratory, USA, [4]CIC Energigune, Spain, [5]Universidad de Santiago de Compostela, Spain

Heat management is one of the major challenges in the development of a wide range of novel technologies [1]. It is thus important to be able to predictively model heat transport ab-initio, in generic multi-scale material structures which may include novel compounds. This is the goal of the Alma project (www.almabte.eu). Here we will discuss various aspects that require a specific theoretical treatment beyond standard approaches. We will present calculations of the cross plane thermal conductivity of crystalline and solid solution thin films, including SiGe, InGaAs, AlGaN, and the highly anisotropic SnSe [2], unveiling the existence of a distinct fractional thickness dependence regime for alloys. We will also show the effect of vacancies on the thermal conductivity of boron arsenide - which has recently been identified as a potential competitor of diamond as a heat sink material [3]. We will then discuss the necessary quadratic nature of the lowest phonon dispersion mode in 2D materials, illustrating it in the case of “borophene” [4]. Finally, we will explain how temperature dependent phonon dispersions, and soft modes in particular, lead to negative thermal expansion, and anomalous thermal conductivity, in empty perovskite ScF3 [5].

[1] D. G. Cahill et al., Appl. Phys. Rev. 1, 011305 (2014).
[2] Bjorn Vermeersch, Jesús Carrete, Natalio Mingo, arXiv:1512.01354
[3] L. Lindsay, D. A. Broido, T. L. Reinecke, Phys. Rev. Lett. 111, 025901(2013)
[4] J. Carrete, Wu Li, L. Lindsay, D. A. Broido, L. J. Gallego, N. Mingo, arXiv:1601.02884
[5] Ambroise van Roekeghem, Jesús Carrete, Natalio Mingo, http://arxiv.org/abs/1601.00561

(B4 oral) **Thermoelectric properties of half-Heusler heterostructures from first-principles calculations**

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University Duisburg-Essen, Germany

Semiconducting half-Heusler alloys have recently emerged as a class of thermoelectric materials with outstanding performance in the medium-to-high temperature range. Heterostructures promise further reduction of the thermal conductivity due to phonon scattering at interfaces. Here, both the electronic and the phononic spectra of half-Heusler compounds based on Ti, Zr, and Hf are calculated using density functional theory (DFT). With this input, thermoelectric properties such as the Seebeck coefficient and the power factor are obtained.

We demonstrate how the thermal conductivity of a superlattice can be estimated in dependence on its period, by using the mean free path of phonons in bulk materials plus an extension of the diffuse mismatch model of phonon transport through the interface. The results are compared to experiment (PRB 92 (2015), 125436). Moreover, superlattices formed by combining Ni-based and Co-based half-Heusler alloys are considered. We demonstrate that, in a short-period superlattice, a high power factor may be retained, while the thermal conductivity is much reduced compared to single-phase half-Heusler crystals. We also address the physics of point defects in both Ni-based and Co-based materials. While interstitial Ni atoms have low formation energy in the Ni-based material and can be used for self-doping, the Co-based material shows high formation energy for Co interstitials and vacancies.

(B4 oral) **Ab initio calculations of the lattice thermal conductivity and the discovery of new thermoelectric materials**

L Chaput[1], A Togo[2], A Seko[2], H Hayashi[2], K Tsuda[2], M Amsler[3], S Goedecker[4], D Lacroix[5] and I Tanaka[2]

[1]Université de Lorraine, France, [2]Kyoto University, Japan, [3]Northwestern University, USA, [4]Basel University, Switzerland, [5]Lorraine University, France

Within the last few years it has been possible to compute the lattice thermal conductivity of bulk materials using ab initio methods. The interactions between the phonons are obtained from density functional theory and this information is incorporated into the Boltzmann to obtain the thermal conductivity. The good accuracy obtained from those calculations allows trying to use to find new materials. We present several strategies that we used performing such a search.

The first method we used is datamining. We screened the entire MPD library to find materials with ultra low thermal conductivity using a Bayesian algorithm based on kriging with gaussian regression processes. We were able to evidence new crystalline structures, some of them with a thermal conductivity lower than wood! Among these compounds some have good electronic properties that could make them exceptional thermoelectric materials.
The second method we used is based on polymorphism. Starting from the experimentally known crystalline phase of the thermoelectric Zn-Sb compound, we reconstructed the energy surface using the Minima Hopping Method and discovered that the ground state is not the experimentally known phase. Computing the physical properties we realized that this new ground state has even better thermoelectric properties than the known ZnSb phase.
Finally we conclude showing how ab initio calculations can be combined with Monte Carlo simulations of the Boltzmann equation. This approach allows describing thermal conduction at the micron scale, and can therefore be used to study nanostructured materials useful for thermoelectric applications.

(B4 oral) **Calculating thermal conductivity using the quasi-harmonic approximation**

G Madsen[1] and R Stern[2]

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Based on the original work by Slack[1], it is shown how the lattice thermal conductivity can be rapidly screened based on the quasi harmonic approximation.[2] The model is validated on a high-throughput dataset and the good performance is related to the definition of the mode-averaged Grüneisen parameter.[3] The thermal conductivity of complex structures such as ZnSb and Zn4Sb3[1] will be discussed and it will be shown how an atomic understanding of the very low thermal conductivity of Zn4Sb3 can be obtained.

The model opens for the high-throughput calculation of thermal conductivity. Two failures of the model[4,5] will be analysed and a mathematically more rigorous version will be introduced. It is shown how the three phonon phase space can be included and the model can be systematically improved.

[1] G. A. Slack, Solid State Phys. 34, 1 (1979)
[2] L. Bjerg et al Phys. Rev. B., 89 024304 (2014)
[3] G. K. H. Madsen et al DOI: 10.1002/pssa.201532615
[4] A. Katre et al J. Appl.Phys. 117, 045102 (2015)
[5] L. Lindsay et al., Phys. Rev. Lett. 111, 025901 (2013)

(B5 invited) **Intermediate models for bridging from high-throughput data to materials properties**

R Drautz

ICAMS, Germany

The relative ease with which reliable high-throughput density functional theory (DFT) calculations may be carried out today and the availability of high-throughput data in large databases forms a solid foundation from which modellers may contribute to the design of new materials. For many materials properties of interest, however, the data in current databases is insufficient because the processes of interest are to complex or take place on a length or time scales that are beyond DFT. Then the high-throughput data merely provides information for the parameterization of intermediate models from which the properties of interest may be predicted.

In this talk I will discuss two classes of intermediate models that we use in our research. Lattice based models will be briefly introduced and discussed for estimating the free energy of competing phases in battery materials. Coarse grained models of the electronic structure will be derived and applications to modelling dislocation - carbon interactions in iron will be discussed. The coarse grained models of the electronic structure will then be stripped down to few essential parameters and the relevance of these parameters for phase stability in sp-d compounds as well as high-entropy alloys will be highlighted.

The computational efficiency of intermediate models as compared to DFT furthermore allows for a systematic coarse graining of simulation time and therefore enables the computation of rare event dynamics solely from the interatomic interaction. An outlook will be given for the prediction of the kinetics of solid-solid phase transformations from atomistic simulations.

(B5 oral) **Combining the many-body GW and Bethe-Salpeter formalisms with polarizable continuum or discrete models**

X Blase[1], J Li[1], I Duchemin[2], G D'Avino[3], D Jacquemin[4] and D Beljonne[3]

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The study of the electronic properties of molecular systems, for applications in (opto) electronics, wet chemistry or biology, represents a formidable challenge for ab initio calculations. There has been recently much interest in the use of specific many-body perturbation theories, the GW and Bethe-Salpeter formalisms, for the study of the electronic and optical properties of organic systems. Recent benchmark studies have shown that such techniques provide the spectrum of charged and neutral excitations [1-2] of organic molecular systems with excellent accuracy as compared to experiment or reference calculations, with a reasonable O(N^4) scaling allowing to treat a few hundred atoms. In particular, the standard problem of charge transfer excitations can be easily handled [3-4]. We will present recent developments for the merging of the GW and Bethe-Salpeter formalisms with the Polarisable Continuum Model (PCM), with applications to hydrated nucleobases, and with discrete induced-charge and dipoles micro-electrostatic models [6], with applications to doped organic semiconductors. Such developments are part of the Fiesta initiative, a massively parallel Gaussian-bases GW and Bethe-Salpeter code.

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[1] X. Blase et al., Phys. Rev. B 83, 115103 (2011)
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[3] I. Duchemin et al., Phys. Rev. Lett. 109, 167801 (2012)
[4] D. Niedzialek et al., Adv. Funct. Mater. 25 pp. 1287-1295 (2015)
[5] G. D'Avino et al., J. Chem. Theory Comput. 10, pp 4959–4971 (2014)

(B5 oral) **Materials design of a room-temperature maser**

S Bogatko, A Horsfield, P Haynes and M Oxborrow

Imperial College London, UK

The maser is the microwave analogue of the laser, well-known for enabling high-quality amplifiers. To date the maser has been limited in application due to the high vacuum and low temperatures needed for it to function. A maser capable of operating continuously under ambient conditions without large magnetic fields, vacuum pumps and cryogenic cooling systems would revolutionise the domains of microwave communication and electron paramagnetic resonance spectroscopy by enabling high precision measurements, such as for biological structure determination. Significant progress was made with the invention of a pentacene/*p*-terphenyl based organic maser that operates at room temperature in pulsed mode[1]. Here we present a computational molecular design study to guide the search for active molecules for a room-temperature maser with an emphasis on finding materials for continuous-wave operation. We focus on linear polyacenes and their diaza-substituted forms and model how important maser properties are influenced by acene length and location of nitrogen substitution. We find that tetracene, its diaza-substituted forms and anthracene possess singlet to triplet intersystem crossing rates highly favourable towards masing. The diaza-substituted forms of pentacene also stand out as ideal candidates due to their similarity to the working pentacene prototype. A steady-state population analysis suggests the working conditions under which continuous-wave masing can be achieved.

[1] M. Oxborrow, J. Breeze and N. Alford, *Nature*, 2012, 488, 353

(B5 oral) **Molecular origin of the charge carrier mobility in small molecule organic semiconductors**

W Wenzel[1], P Friederich[2], V Meded[2], T Neumann[2], F Symalla[2], V Rodin[3] and F von Wrochem[3]

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Small-molecule organic semiconductors are used in a wide spectrum of applications, ranging from organic light emitting diodes to organic photovoltaics. However, the low carrier mobility severely limits their potential, e.g. for large area devices. A number of factors determines mobility, such as molecular packing, electronic structure, dipole moment and polarizability, however these molecule-dependent determinants are hard to disentangle. Here, we present a parameter-free model, which provides an accurate prediction of experimental data over ten orders of magnitude in mobility, and allows for the decomposition of the carrier mobility into molecule-specific quantities. We also demonstrate that a single molecular property, *i.e.* the dependence of the orbital energy on conformation, is the key factor defining mobility for hole transport materials. The availability of first-principles models to compute key performance characteristics of organic semiconductors may enable in-silico screening of numerous chemical compounds for the development of highly efficient opto-electronic devices.

(P2.01) **Spectral transmission at cubic Ge/hexagonal Ge interface: Molecular dynamics vs "full-band" mismatch model**

B Davier[1], J Larroque[1], T Kaewmaraya[1], L Chaput[2], Y Chalopin[3], P Dollfus[1], S Volz[3] and J Saint-Martin[1]

[1]Université Paris Sud, France, [2]Université de Lorraine, France, [3]Ecole Centrale Paris, France

The development of today's Information and Communication Technologies is strongly related to the thermal management of nanoelectronic and optoelectronic systems. Thermoelectric conversion constitutes a solution to optimize cooling and energy reconversion. The recent trend in the optimization of thermoelectricity lies in the manipulation of thermal properties via nanostructures such as nanowires. Germanium polytypes nanowires have been recently fabricated experimentally. They exhibit a periodic alternation of cubic and hexagonal Germanium phases, and the resulting interfaces are expected to decrease drastically thermal conduction without degrading too much the electron transport, thus increasing the conversion efficiency.

In this work, Molecular Dynamics simulations are performed in order to study the thermal properties of the nanowire from the recovery of the time dynamics of atomic nucleus. Then, the interface between cubic and hexagonal phases is simulated for several orientations in order to extract the interfacial thermal resistances and the phonon spectral transmissions. These spectral transmissions are compared with several transmissions computed within a "Full-band" Mismatch Model (MM). To compute "Full-band" phonon dispersions Adiabatic Bond Charge Model and DFT calculations are used and compared. In the next step, these dispersions and transmissions have to be included in a Monte-Carlo method for phonon transport to simulate the complete nanowire.

(P2.02) **Origin of subgap states in amorphous transparent (semi-)conducting oxides**

W Körner, D Urban and C Elsässer

Fraunhofer IWM, Germany

The influences of atomic defects and structural disorder on thermodynamic and electronic properties of amorphous indium based (IGZO, ITO, IZO), indium-free (ZTO) and related oxides are investigated by density-functional-theory (DFT) calculations with supercell models containing atomic and extended defects. For vacancies, cation dopants substituting Zn or Sn, and anion dopants substituting O as atomic defects, defect levels in the electronic band structures are analysed in terms of densities of states, which are calculated by means of the LDA with a self-interaction-correction (SIC). The important outcome of this study is detailed microscopic information on how much positions and shapes of electronic defect levels can be altered in amorphous structures with respect to doped single crystals. Based on our extensive set of DFT results for In-, Sn-, Zn- based oxides we develop a general concept of the subgap states which is applicable to these systems. Our results [1-3] support experimental efforts to control the emergence of detrimental subgap states and thereby tune the material properties, either through the choice of appropriate growth conditions or by applying additional post-growth treatments

[1] Körner, Urban, und Elsässer, Origin of subgap states in amorphous In-Ga-Zn-O, J. Appl. Phys. 114, 163704 (2013)
[2] Körner and Elsässer, DFT study of stability and subgap states of crystalline and amorphous Zn-Sn-O, Thin Solid Films 555, 81-86 (2014)
[3] Körner, Urban and Elsässer, Generic origin of subgap states in transparent amorphous semiconductor oxides illustrated for the cases of In-Zn-O and In-Sn-O, Phys. Status Solidi A 212, 1476–1481 (2015)

(P2.03) **The martensitic transformation in Ti-Ta high temperature shape memory alloy: Insight from first principles calculations**

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Shape memory alloys (SMAs) that can be used at high-temperature (> 373 K) are an important class of materials for automotive, aviation and biomedical applications. The transformation temperature as well as mechanical properties of these alloys are usually strongly composition dependent. First principles calculations can provide fundamental insight into the composition dependent transformation temperature as well as transformation mechanism.

One of the key quantities that determine the transformation temperature is the free energy of the involved crystal phases as a function of temperature and composition. Using density functional theory (DFT) one may evaluate the different contributions to the free energy to compare the phase stability at finite temperature.

In Ti-Ta the martensitic transformation temperature between the cubic austenite and orthorhombic martensite exhibits a linear dependence on the composition. Using special quasi-random structures to model the chemical disorder we show that this behaviour is well captured by the relative phase stability at T=0K. We systematically extend our DFT study to include finite temperature contributions. Screening the entire composition range we identify trends that may aid the design of SMAs with targeted transformation temperatures and elastic properties.

(P2.04) **Multi-scale modelling to relate Be surface temperature, D concentration and molecular sputtering yields in future fusion reactors**

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[1]University of Helsinki, Finland, [2]University of Madrid, Spain, [3]Oak Ridge National Laboratory, USA

The success of ITER highly depends on understanding the interplay between the plasma particles and the wall components. Since its main wall will be made of beryllium (Be), knowing the relationship between Be surface temperature, deuterium (D) concentration and Be erosion as well as identifying the sputtered species and underlying mechanisms, is essential. All this will assist in both assessing the wall life-time and making reliable predictions about the plasma impurity transport and related redeposition patterns.

The experiments provide a broad database for the erosion yields, but unfortunately they do not provide complete information about the complex relationship of surface temperature with D concentration at the surface.

However, more accurate beryllium deutride molecular erosion yields can be computed using a molecular dynamics and object kinetic Monte Carlo (MD-OKMC) multiscale approach, allowing more precise accounting of the complex relationship with and between surface temperature and D concentration. In this work, first we used OKMC technique to determine equilibrium D profiles in Be varying vacancy concentration and surface temperature. Then, the D and vacancy profiles from OKMC were then used to set-up accurate substrate structure for MD simulations. In MD cells, D atoms were implanted according to depth profiles given by OKMC. Be-D molecular erosion yields were studied by irradiating the mentioned created cell with D with energies 10-200 eV, scanning over different temperatures (300-800K).

Our OKMC results show that there is almost linear dependence between D concentration and vacancy concentration while surface temperature has a significant effect on D depth profile.

(P2.05) **High-throughput search for topological crystalline insulators**

H Lee and O V Yazyev

Ecole Polytechnique Fédérale de Lausanne (EPFL), France

Topological order in condensed matter has one-to-one correspondence with underlying symmetry, which ensures its stability against symmetry-preserving perturbations. In principle, for every discrete symmetry, there must exist topological insulating phases and corresponding topological quantum numbers, which classify these phases. Among them, crystal symmetry has been regarded as another fertile ground for exploring nontrivial topological phase due to its diversity and complexity. In this work, we perform high-throughput search for crystal-symmetry-protected topological insulators, dubbed topological crystalline insulators (TCIs). In particular, we consider TCI phases protected by mirror symmetry or non-symmorphic glide reflection symmetry. For this purpose, we calculate the mirror Chern number and the topological winding number by using the efficient discretized form of Berry curvature and Berry phase with the Wilson loop approach. Furthermore, in order to make this search more efficient, we exploit the little group of Bloch states and parallelize the calculation of topological numbers. The developed methodology is fully integrated into ab initio codes at the level of (semi)local density-functional theory (DFT) and extended to the advanced approaches beyond DFT such as hybrid functional and GW approximation. Along with the computational flow with the core ingredients, we report the results on some candidates for topological crystalline insulators.

(P2.06) **Systematic search for lithium ion conducting compounds by screening of compositions combined with atomistic simulation**

D Mutter[1], B Lang[1], B Ziebarth[2], C Elsässer[3] and G Krugel[4]

[1]Albert-Ludwigs-Universität Freiburg, Germany, [2]Karlsruher Institut für Technologie , Germany, [3]Technologie, Institut für Angewandte Materialien (IAM-CMS), Germany, [4]Ludwigs-Universität Freiburg, Germany

Solid state electrolytes (SSEs) with high Li conductivity could significantly improve Li ion accumulators in terms of electrochemical efficiency, thermal and mechanical stability, and environmental compatibility, leading to an enhanced range of applications for these high energy density batteries.

Compounds crystallizing in the structure of NaZr2(PO4)3 (NZP) are regarded as promising SSEs, mainly because of their three-dimensional diffusion network enabling fast transport of Li ions through well-defined channels.

Starting from LiTi2(PO4)3, we analysed a huge variety of NZP materials by systematically screening the relevant parts of the periodic table, replacing Ti partially and fully by tri-, tetra-, and pentavalent atoms, as well as the phosphate by silicate, vanadate, and arsenate anions.

The influence of different elements on preferred Li sites, Li mobility, and possible diffusion paths were analysed by means of a combined approach of multiple computational methods with different levels of accuracy, ranging from density functional theory to molecular dynamics simulations with ionic bond valence potentials. Minimum energy paths and diffusion barriers were identified by making use of the nudged elastic band method, as well as saddle point and energy landscape calculations.

For LiX2(PO4)3 compounds we show how this screening approach led to clear structure-property relations between the volume of coordination polyhedra around the mobile ions and the corresponding vacancy mediated diffusion barriers. Additionally, an interstitial migration mechanism was identified with a migration barrier which is significant lower than that of the vacancy diffusion, which may explain an experimentally reported change in the diffusion mechanism at elevated temperatures.

(P2.07) **Charge transport in OLED guest host systems: The role of molecular superexchange**

F Symalla[1], P Friederich[1], V Meded[1], A Masse[2], P Bobbert[2] and W Wenzel[1]

[1]Karlsruhe Institute of Technology, Germany, [2]Technical University Eindhoven, Netherlands

Organic light emission diodes (OLEDs) are a class of organic electronics widely used in state of the art display technologies. Hopping charge transport in multi component OLED materials, in particular guest host layers is not yet fully understood. We show that charge transport in guest host layers of OLEDs is enhanced significantly by virtual hopping processes through intermediate molecules. The hopping range of charges in energy traps is increased by virtual hops, facilitating hopping from trap to trap at lower guest concentrations than direct hopping would allow, as the effective coordination of trap states is considerably modified. This has impact on rational material design which seeks to optimize emitter concentration with respect to the trade-off between exciton trapping and charge mobility.

(P2.08) **First principles investigation of the magneto-electric properties into Yttrium and Gallium orthoferrite**

D Stoeffler

CNRS-IPCMS (DMONS), France

Magneto-electric materials are particularly interesting because of their coupled electric polarization and magnetization. This allows to expect to act on the magnetism using an electric field (and reciprocally): for example, less power consuming reversal of a magnetic domain state could be operated with assistance of an applied voltage.

The investigation of the origin of the magneto-electric coupling with first principles approaches remains challenging because very small variations have to be determined taking the spin-orbit coupling into account. Three contributions to magneto-electricity are usually considered: purely electronic (frozen atomic positions), lattice mediated (atomic displacement into a frozen cell) and stress induced (unit cell deformation). The present work aims to determine the magnetic and dielectric properties of orthoferrite systems (namely GaFeO3 and YFeO3) and their coupling using the first principles Projector Augmented Wave method implemented into the VASP code.

It is shown that GaFeO3 presents a large polarization of 0.25 C/m2 due to its Pna21 polar structure but, being antiferromagnetically ordered, presents no net magnetization without Fe-Ga chemical disorder. In order to investigate the magneto-electric coupling from a purely electronic viewpoint, the variations of the polarization induced by varying the magnetic configuration are determined and discussed.

It is also shown that YFeO3, having a centrosymmetric Pnma structure, presents no net polarization but, its antiferromagnetic order being canted, its magnetization exhibits a small ferromagnetic component of 0.05 μB per Fe atom. In order to break the inversion symmetry, small atomic displacements are considered to investigate the lattice mediated magneto-electric coupling.

(P2.09) **Exploring the real ground-state structures of molybdenum dinitride**

B Huang[1], S Yu[2], Q Zeng[2], A Oganov[3] and G Frapper[4]

[1]Université de Poitiers - CNRS, France, [2]Northwestern Polytechnical University, China, [3]Moscow Institute of Physics and Technology, Russia, [4]Université de Poitiers - CNRS, France

Transition metal nitrides play an important role in catalysis. Molybdenum dinitride (MoN2) was recently synthesized at a moderate pressure of 3.5 GPa and a layered MoS2-type structure has been proposed [1]. However, the thermodynamic, mechanical and dynamical properties based on DFT calculations suggest that this layered R3m structure is unstable [2]. Therefore, stable structures of MoN2 at pressures from atmospheric pressure up to 100 GPa have been further examined by using USPEX code based on an evolutionary algorithm which mimics Darwinian evolution. We find a pernitride structure with space group P63/mmc which is the ground state of the MoN2 system. It transforms to a P4/mbm phase above 82 GPa. Chemical bonding analysis shows that one could assign MoN2 as Mo4+(N24-), i.e. Mo is formally a d2 metal. The presences of covalent N2 dumbbells and strong bonding between Mo4+ and N24- are the source of the superior mechanical properties of these predicted ultra-incompressible or ultra-hard MoN2 pernitrides.

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[2] Yu, S.; Huang, B.; Jia, X.; Zeng, Q.; Oganov, A.; Zhang,L.; Frapper, G.; J. Phys. Chem. C, 2016, 120 (20), pp 11060–11067

Symposium C

(C1 invited) **Coarse graining interatomic potentials with machine learning**

G Csanyi

University of Cambridge, UK

Machine learning methods are extensively being tried as a means of deriving accurate interatomic potentials from electronic structure calculations. Although one could argue that the electronic degrees of freedom are being eliminated in this step, this is not strictly true, since the target function is the Born-Oppenheimer potential energy surface (BO-PES), and although when calculating its values we use electronic structure calculations, the BO-PES is already defined only in terms of the atomic degrees of freedom as its variables. Here we apply machine learning (in the form of the Gaussian Approximation Potentials, GAPs) to do true coarse graining (CG): learning free energies of molecules as a function of their conformations, and demosntrate that much better accuracy can be obtained than with traditional pair-potential CG approaches.

(C1 oral) **Active learning of interatomic potentials**

A Shapeev and E Podryabinkin

Skolkovo Institute of Science and Technology, Russia

Interatomic potentials are usually fitted on a database of experimental data or ab initio calculations. In the latter case, the database is often obtained prior to fitting and contains relevant (to the problem at hand) atomistic configurations together with their energies and interatomic forces. However, for accurate potentials with many unknown coefficients, obtaining a suitable database becomes a separate problem.

This work considers the problem of an automated creation of the database for a given form of the potential. To that end, we formulate an algorithm that selects the best atomistic configurations for fitting, based on a variance-reduction-type criterion. One obvious application of this is learning on the fly (semi-supervised learning), i.e., fitting the potential while running a single molecular-dynamic trajectory. Another application is the offline database creation (unsupervised machine learning). In our presentation we will expose our algorithm and report on its performance.

(C1 oral) **QM/MM coupling for crystalline defect simulations**

H Chen and C Ortner

University of Warwick, UK

QM/MM coupling is a widely used technique to perform atomistic simulations of large systems as encountered in materials science and biochemistry. In the context of materials science, the regions of interest such as a defect core, is modelled by an electronic structure model, while the material bulk is modelled with a computationally inexpensive interatomic potential model. We analyse a minimalist electronic structure model: the tight-binding model, and present a new type of locality result. Exploiting this locality, we construct a QM/MM coupling scheme based on energy mixing, where the MM potential can couple well with the QM model. The efficiency and accuracy of this construction are shown by rigorous analysis and numerical experiments.

(C1 oral) **Mathematical modeling of incommensurate 2D materials**

M Luskin

University of Minnesota, USA

Incommensurate materials are found in crystals, liquid crystals, and quasi-crystals. Stacking a few layers of 2D materials such as graphene and molybdenum disulfide, for example, opens the possibility to tune the elastic, electronic, and optical properties of these materials. One of the main issues encountered in the mathematical modeling of layered 2D materials is that lattice mismatch and rotations between the layers destroys the periodic character of the system. This leads to complex commensurate-incommensurate transitions and pattern formation.

Even basic concepts like the Cauchy-Born strain energy density, the electronic density of states, and the Kubo-Greenwood formulas for transport properties have not been given a rigorous analysis in the incommensurate setting. New approximate approaches will be discussed and the validity and efficiency of these approximations will be examined from mathematical and numerical analysis perspectives.

(C2 invited) **Model order reduction techniques for numerical homogenization**

A Abdulle

EPFL, Switzerland

In this talk we discuss the combination of numerical homogenization techniques (a class of multiscale methods) with reduced order modelling techniques such as the reduced basis method for the efficient solution of partial differential equations with multiple scales. Applications to linear and nonlinear heat conduction in heterogeneous material and flow problems in porous media will be discussed.

The results presented are based upon a series of joint works with various collaborators (see the references below).

[1] A. Abdulle, Y. Bai, G. Vilmart, Reduced basis finite element heterogeneous multiscale method for quasilinear elliptic homogenization problems. Discrete Contin. Dyn. Syst., 8 (2015), pp. 91-118

[2] A. Abdulle, P. Henning, A reduced basis localized orthogonal decomposition, J. Comput. Phys., 295 (2015), pp. 379-401

[3] A. Abdulle, O. Budac, An adaptive finite element heterogeneous multiscale method for Stokes flow in porous media, SIAM, Multiscale Model. Simul., 13 (2015), pp. 256–290

[4] A. Abdulle, O. Budac, A Petrov-Galerkin reduced basis approximation of the Stokes equation in parametrized geometries, C. R. Math. Acad. Sci. Paris, 353 (2015), pp. 641–645

[5] A. Abdulle, O. Budac, A reduced basis finite element heterogeneous multiscale method for Stokes flow in porous media, to appear in Comput. Methods Appl. Mech. Engrg. (2016)

(C2 oral) **Control of oscillators, temporal homogenization, and energy harvest by super-parametric resonance**

M Tao[1] and H Owhadi[2]

[1]Georgia Institute of Technology, USA, [2]California Institute of Technology, USA

We show how to control an oscillator by periodically perturbing its stiffness, such that its amplitude follows an arbitrary positive smooth function. This also motivates the design of circuits that harvest energies contained in infinitesimal oscillations of ambient electromagnetic fields. To overcome a key obstacle, which is to compensate the dissipative effects due to finite resistances, we propose a theory that quantifies how small/fast periodic perturbations affect multidimensional systems. These result in the discovery of a mechanism that we call super-parametric resonance, which reduces the resistance threshold needed for energy extraction based on coupling a large number of RLC circuits.

(C2 oral) **Numerical homogenization based fast solver for PDEs with arbitrarily rough coefficients**

L Zhang[1] and H Owhadi[2]

[1]Shanghai Jiao Tong University, China, [2]Caltech, USA

Numerical homogenization concerns the finite dimensional approximation of the solution space of, for example, divergence form elliptic equation with L^\infty coefficients which allows for nonseparable scales. Standard methods such as finite-element method with piecewise polynomial elements can perform arbitrarily badly for such problems. Recently, we have proposed a localization approach for numerical homogenization which precomputes H^{-d} localized bases on patches of size H \log(1/H). The localization is due to the exponential decay of the corresponding fine scale solutions with Lagrange type constraints. Interestingly, this approach can be reformulated as a Bayesian inference or decision theory problem. The numerical homogenization method can be used to construct efficient and robust fine scale fast solver such as multigrid solver or multiresolution decomposition with bounded condition number on each subband, and generalized to time dependent problems such as wave propagation in heterogeneous media.

(C2 oral) **The local orthogonal decomposition method for problems with complex geometry**

D Elfverson[1], A Målqvist[2] and M Larson[1]

[1]Umeå University, Sweden, [2]Chalmers University of Technology and University of Gothenburg, Sweden

In this paper we extend the local orthogonal decomposition multiscale method [1] to elliptic problems on complex domains, e.g. domains with cracks or complicated boundary. We construct corrected coarse test and trail spaces which takes the fine scale features of the domain into account. The corrections only need to be computed in regions affected by the fine scale geometrical information of the domain. We achieve linear convergence rate in energy norm for the multiscale solution. Moreover, the conditioning of the multiscale method is not affected by how the domain boundary cuts the coarse elements in the background mesh. We present a series of numerical experiments which verifies the analytical findings.

[1] A. Målqvist and D. Peterseim. *Localization of elliptic multiscale problems.* Math. Comp., 83(290):2583–2603, 2014

(C2 oral) **From the Newton equation to the wave equation in case of shocks**

M Josien[1] and X Blanc[2]

[1]ENPC, France, [2]LJLLL, France

It has been recently proved by X. Blanc, C. Le Bris and P.-L. Lions that one can derive the wave equation from a chain of numerous particles submitted to the Newton equations (each particle interacting through a potential with its nearest neighbours). However, the assumptions necessary for this derivation forbid any shock wave, whereas nonlinear wave equations tend to create shocks for almost every smooth initial data. Therefore, with X. Blanc, we tried to understand the specific phenomena involved in shock, for linear and non-linear potentials. Surprisingly enough, we discovered that in the linear case, the Newton equations still tend to the wave equation whether there are shocks or not, but that this is false for a large class of non-linear convex potentials as soon as there is a shock: in this case, one can observe dispersive shock waves (which is well-known in the case of Toda lattice). Thus, in that non-linear convex cases, an atomic chain submitted to the Newton equations can be well described by the wave equation until a shock, and then this approximation becomes false. In this talk, I give a few ingredients of the proof, which requires anyway a conjecture unproved until now.

(C3 invited) **Kinetic modeling of materials coarsening: from individual grains to network statistics**

M Emelianenko

George Mason University, USA

When microstructure of polycrystalline materials undergoes coarsening driven by the elimination of energetically unfavorable crystals, a sequence of network transformations, including continuous expansion and instantaneous topological transitions, takes place. This talk will be focused on recent advances related to the mathematical modeling of this process. Two types of approaches will be discussed, one aimed at simulating the evolution of individual crystals in a 2-dimensional system via a vertex model focused on triple junction dynamics, and one providing a kinetic Boltzmann-type description for the evolution of probability density functions. The predicted MDF evolution based on the new kinetic mesoscale model will be discussed and contrasted with those obtained by large-scale phase field, MC and vertex simulations for several classes of interfacial energies.

(C3 oral) **Stochastic model for dislocation climb**

Y Xiang[1], X Niu[1] and J Lu[2]

[1]Hong Kong University of Science and Technology, Hong Kong, [2]Duke University, USA

Dislocation climb mechanism plays an important role in the plastic deformation of crystals at high temperature. In the climb motion, dislocations change slip planes by absorbing or emitting vacancies. This process is coupled with vacancy diffusion and becomes significant at high temperatures. A stochastic model for the vacancy diffusion assisted dislocation climb will be presented.

(C3 oral) **On the temporal coarse graining in dislocation dynamics**

A El-Azab

Purdue University, USA

Theoretical efforts on coarse graining of dislocation ensembles have recently yielded the first prediction of self-organized dislocation patterns in crystals (S. Xia and A. El-Azab, Modelling Simul. Mater. Sci. Eng. 23 (2015) 055009). These efforts aim to develop density-based models that capture the critical physics of the underlying discrete dislocation system. While most work in this area focuses on spatial coarse graining, some recent pieces of work started to address the question of time coarse graining. Here, we tackle this question by focusing on the rate processes associated with dislocation dynamics, e.g., cross slip and dislocation reaction rates. The concepts of marked point process and time series are used to analyse the statistical properties of these processes in both time and frequency domains. The statistical data required to perform this analysis is obtained using the method of dislocation dynamics simulation. The temporal correlations and correlation times of cross-slip and short-range reactions have been computed. It is found that the correlation time for cross-slip is the largest of all correlation times and, as such, it is considered here to be the coarse graining time-scale in continuum dislocation dynamics. Using this mesoscopic time-scale, a coarse grained stochastic representation of cross slip and dislocation reactions has been achieved and implemented in continuum dislocation dynamics to predict the self-organized dislocation patterns.

(C3 oral) **Generic adaptive resolution approach to reverse mapping of polymer melts**

J Krajniak, G Samaey, S Pandiyan and E Nies

KU Leuven, Belgium

Over the past two decades, coarse-grained (CG) simulation has become an important method that allows exploring behaviour of larger (bio-)polymer systems over longer time scales. Although many properties of polymers can be analysed at the CG level, some properties strictly depend on the presence of fine-scale degrees of freedom. Therefore, there is a demand for a computational tool that reintroduces atomistic details in an already performed coarse-grained simulation.

In this contribution, we present a generic method of reverse mapping that is based on the adaptive resolution scheme (AdResS)[1]. In AdResS simulation, one brings together two spatial domains, modelled at two different scales, in a concurrent simulation. This is done by defining a hybrid region where, by the *spatial-dependent* switching function, particles change from the coarse-grained to the atomistic resolution. We use this method from a different perspective by treating a whole simulation box as a hybrid region and using the *time-dependent* switching function. Additionally, we introduce bonded potentials that scale with changing resolution. This approach prevents the introduction of a huge potential energy that could arise in the early stage where the resolution is close to the coarse-grained. We use our method to reconstruct polymer melts and complex polymer networks from the coarse-grained to the all-atom state. We compare conformational and dynamical properties of reconstructed systems with the reference atomistic simulation.

[1] M. Praprotnik, L. Delle Site, and K. Kremer, “Adaptive resolution molecular-dynamics simulation: Changing the degrees of freedom on the fly,” J. Chem. Phys., vol. 123, no. 200

(C4+F4 oral) **Multiscale modelling of materials chemomechanics**

J Kermode

University of Warwick, UK

The requirements for modelling chemomechanical processes such as fracture which are strongly coupled across lengthscales [1] can be met simultaneously by combining a quantum mechanical description of regions of interest (e.g. crack tips or dislocation cores) with a classical atomistic model that captures the long-range elastic behaviour using a QM/MM (quantum mechanics/molecular mechanics) approach such as the `Learn on the Fly' (LOTF) scheme [2,3]. Applications of the technique will be presented, e.g. interactions between moving cracks and material defects such as dislocations or impurities [4], very slow crack propagation via kink formation and migration [5] and chemically activated fracture, where cracks advance under the concerted action of stress and corrosion [6]. The expansion of the approach to metals will be reported through an ongoing application to dislocation motion in Ni-based superalloys [7].

[1] E. Bitzek, J. R. Kermode and P. Gumbsch, Atomistic aspects of fracture, Int. J. Fract. 191, 13-30 (2015)
[2] G. Csányi, T. Albaret, M. Payne and A. De Vita, Phys. Rev. Lett. 93, 175503 (2004)
[3] Z. Li, J. R. Kermode, and A. De Vita, Phys. Rev. Lett. 114, 096405 (2015)
[4] J. R. Kermode, et al., Nat. Commun. 4, 2441 (2013)
[5] J. R. Kermode, A. Gleizer, G. Kovel, L. Pastewka, G. Csányi, D. Sherman, and A. De Vita, Phys. Rev. Lett. 115, 135501 (2015)
[6] A. Gleizer, G. Peralta, J. R. Kermode, A. De Vita and D. Sherman, Phys. Rev. Lett. 112, 115501 (2014).
[7] F. Bianchini, J. R. Kermode and A. De Vita, Submitted (2016)

(C4+F4 oral) **Uncertainty quantification across the DFT/MD scale boundary in sequential multiscale simulations**

P Brommer

University of Warwick, UK

Density functional theory (DFT) simulation methods are a cornerstone of materials modelling: New modelling techniques, algorithmic improvements and ever more powerful computers have made *ab-initio* simulations possible on an unprecedented scale across many areas of materials science. On the other hand, "cheap" Molecular Dynamics (MD) simulations with classical effective potentials still have their right to exist (and account for a significant fraction of HPC usage). Simulations with millions of atoms over millions of timesteps - routinely done with classical MD - still are far beyond current DFT capabilities. However, this scale jump comes at a cost: Whereas *ab-initio* methods at least in name are derived from first principles, effective potentials in their standard formulation require the user to make some assumptions and approximations about how the interactions are computed from the positions of the atoms. The consequences of these choices on the quantities of interest are badly controlled, and in most cases the confidence of the final result of a MD simulation is unknown a priori. Usually, the potential is validated by comparing results to DFT after the fact where this is possible, extrapolating into the unknown where it is not.

Here, I present methods to quantify the uncertainties of standard effective potentials in the potential generation process and propagate this uncertainty to the final simulation result, with a particular focus on compatibility with the existing software stack in atomistic modelling. This will allow to equip sequential multiscale simulations with the uncertainty quantification (UQ) required to make them truly predictive.

(C5 invited) **Large-scale real-space electronic structure calculations**

V Gavini and P Motamarri

University of Michigan, USA

In this talk, the development of a real-space formulation for Kohn-Sham density functional theory (DFT) and a finite-element discretization of this formulation [1], which can handle arbitrary boundary conditions and is amenable to adaptive coarse-graining, will be presented. In particular, the accuracy afforded by using higher-order finite-element discretizations, and the efficiency and scalability of the Chebyshev filtering algorithm in pseudopotential and all-electron Kohn-Sham DFT calculations will be demonstrated. Further, the development of a subquadratic-scaling approach (in the number of electrons) based on a subspace projection and Fermi-operator expansion will be discussed [2], which will be the basis for the future development of coarse-graining techniques for Kohn-Sham DFT. The developed techniques have enabled, to date, pseudopotential calculations on non-periodic and periodic systems containing ~10,000 atoms, as well as all-electron calculations on systems containing ~5,000 electrons.

[1] P. Motamarri et al., Higher-order adaptive finite-element methods for Kohn-Sham density functional theory, J. Comp. Phys. 253, 308-343 (2013).

[2] P. Motamarri, V. Gavini, A subquadratic-scaling subspace projection method for large-scale Kohn-Sham DFT calculations using spectral finite-element discretization, Phys. Rev. B 90, 115127 (2014).

(C5 oral) **Automating diffusivity calculations for interstitial and solute diffusion from first-principles**

D Trinkle

University of Illinois at Urbana–Champaign, USA

Mass transport controls crucial materials processing, such as segregation and precipitation, and properties, such as ionic conductivity, in a wide variety of materials. First-principles methods can determine the activated state energies at the atomic level involved in mass-transport such as vacancies moving in a crystal. Upscaling from activation barriers to mesoscale mobilities requires the solution of the master equation for diffusivity. For all but the simplest cases of interstitial diffusivity, and particular approximations with vacancy-mediated diffusion on simple lattices, calculating diffusivity directly is a challenge. This leaves two choices: uncontrolled approximations to map the problem onto a simpler (solved) problem, or a stochastic method like kinetic Monte Carlo, which can be difficult to converge for cases of strong correlations. Moreover, without analytic or semi-analytic solutions, evaluating derivatives of transport coefficients is also difficult. We describe and demonstrate the development of direct and automated Green's function solutions for transport that take full advantage of crystal symmetry. To showcase the new functionality, we consider hexagonal lattices where previous models have been limited. We consider interstitial diffusivity of light elements in magnesium--including the elastodiffusion tensor and activation volume tensor--and vacancy-mediated diffusion of substitutional solute in magnesium. All of these include correlation effects on transport. The underlying automation also makes the extension of first-principles transport databases significantly more practical and eliminate uncontrolled approximations in the transport model

(C5 oral) **The flexibility of daubechies wavelets for electronic structure calculations**

T Deutsch[1], L Genovese[1], S Mohr[2], L Ratcliff[3] and S Goedecker[4]

[1]LSim - Univ. Grenoble Alpes, CEA, INAC, France, [2]CASE Group, BSC, Spain, [3]Argonne National Laboratory, USA, [5]Basel University, Switzerland

Since 2008, the BigDFT project consortium has developed an ab initio Density Functional Theory code based on Daubechies wavelets. These are a compact support multiresolution basis, optimal for expanding localised information, and form one of the few examples of systematic real space basis sets.

In recent articles, we presented the linear scaling version of BigDFT code [1], where a minimal set of localized support functions is optimized in situ. Our linear scaling approach is able to generate support functions for systems in various boundary conditions, like surfaces geometries or system with a net charge. The real space description provided in this way allows to build an efficient, clean method to treat systems in complex environments, and it is based on an algorithm which is universally applicable [2], requiring only moderate amount of computing resources.

We will present how the flexibility of this approach is helpful in providing a basis set that is optimally tuned to the chemical environment surrounding each atom.
In addition than providing a basis useful to project Kohn-Sham orbitals informations like atomic charges and partial density of states, it can also be reused as-is, i.e. without reoptimization, for charge-constrained DFT calculations within a fragment approach [3]. We will demonstrate the interest of this approach to express highly precise and efficient calculations for the computational setup of systems in complex environments [4].

[1] J. Chem. Phys. 140, 204110 (2014)
[2] Phys. Chem. Chem. Phys., 2015, 17, 31360-31370
[3] J. Chem. Phys. 142, 23, 234105 (2015)
[4] J.Chem. Theory Comput. 2015, 11, 2077

(C5 oral) **Wavefunction in DFT embedding for materials design**

S Bogatko and A Horsfield

Imperial College London, UK

Quantum embedding methods have long been known to provide an efficient method of including environmental effects in an otherwise intractable quantum problem. A prominent example is Quantum Mechanics/Molecular Mechanics (QM/MM) embedding where the electron density of the environment is represented by atomic point charges. On a technically higher lever, the quantum problem can be embedded in an environment wherein the electron density is represented by Density Functional Theory (DFT). This allows for explicit representation of the electron density thereby including important effects such as polarization. While the computational costs of DFT are indeed greater than MM they are highly advantageous when compared to a full treatment with advanced wave function (WF) methods. Following the recent development of an efficient WF in DFT method by Manby et al. [1,2] we are developing a stand-alone software package which acts as intermediary between standard WF and DFT software packages. In this talk I will cover the main points of WF in DFT, the efficient algorithm developed by Fred Manby, and introduce the software we are developing to carry out this work. The results of test cases will be presented.

[1] F.R. Manby, M. Stella, J.D. Goodpastor, T.F. Miller, J. Chem. Theory Comput. 2012, 8, 2564−2568
[2] S.J. Bennie, M. Stella, TF. Miller, F.R. Manby, J. Chem. Phys. 143, 024105 (2015)

(C5 oral) **Green's functions for seamless elastic boundaries in atomic-scale calculations**

L Pastewka[1], T Sharp[2] and M Robbins[3]

[1]Karlsruhe Institute of Technology, Germany, [2]University of Pennsylvania, USA, [3]Johns Hopkins University, USA

Modelling interfacial phenomena often requires both a detailed atomistic description of surface interactions and accurate calculations of long-range deformations in the substrate. The latter can be efficiently obtained using an elastic Green's function if substrate deformations are small. We present a general formulation for rapidly computing the Green's function for a planar surface given the interatomic interactions, and then coupling the Green's function to explicit atoms. The approach is fast, avoids ghost forces, and is not limited to nearest-neighbor interactions. The full system comprising explicit interfacial atoms and an elastic substrate is described by a single Hamiltonian and interactions in the substrate are treated exactly up to harmonic order. This concurrent multiscale coupling provides simple, seamless elastic boundary conditions for atomistic simulations where near-surface deformations occur, such as nanoindentation, contact, friction, or fracture. Applications using pair-potentials, the embedded atom method and bond-order potentials are used to illustrate the approach.

(C6 invited) **A parallel implementation of the mixed multiscale finite element method for the simulation of two-phase flows in porous media**

G Enchéry, M A Puscas and S Desroziers

IFPEN, France

The mixed multiscale finite element (MMsFE) method features many advantages for the simulation of two-phase flows in large heterogeneous porous media. Based on the divide and conquer strategy shared by all multiscale methods, its basis functions are calculated by defining cell problems which can be easily solved in parallel. The second interesting property of the method lies in the reduction of the size of the linear system used to solve the pressure equation. This reduction is feasible because of the shape of the basic functions which encompasses the local fine-scale variations of the permeability field. At last, the ability of the MMsFE method to provide a two-scale approximation of the fluxes makes possible to couple it, for instance, with a fine-scale finite-volume scheme for the resolution of the saturation equation.

However, because of the calculation of the fluxes on both grids, we show in this work that a two-level MPI strategy is required when implementing the MMsFE method in parallel. This strategy consists in adapting the calculation resources according to the two main steps of the algorithm which are the calculation of the basis functions and the resolution of the linear system in pressure. Using this approach, results of simulations performed on hydrocarbon reservoir models show that a better scalability can be obtained.

(C6 oral) **Asymptotic Preserving numerical schemes for multiscale parabolic problems**

G Vilmart[1], N Crouseilles[2] and M Lemou[2]

[1]University of Geneva, Switzerland, [2]University of Rennes, France

We consider a class of multiscale parabolic problems with diffusion coefficients oscillating in space at a possibly small scale \varepsilon. Numerical homogenization methods are popular for such problems, because they capture efficiently the asymptotic behaviour as \varepsilon \rightarrow 0, without using a dramatically fine spatial discretization at the scale of the fast oscillations. However, known such homogenization schemes are in general not accurate for both the highly oscillatory regime \varepsilon \rightarrow 0 and the non oscillatory regime \varepsilon \sim 1. In this talk, we introduce an Asymptotic Preserving method based on an exact micro-macro decomposition of the solution which remains consistent for both regimes.

(C6 oral) **A generalized finite element method for linear thermoelasticity**

A Persson

Chalmers University of Technology, Sweden

In this talk I will discuss how the local orthogonal decomposition techniques can be used to define a generalized finite element method (GFEM) for linear thermoelasticity equations with spatial multiscale coefficients. The problem is a coupled system consisting of an elliptic equation for elasticity and a parabolic equation for the temperature. Hence, two different decompositions, one for each equation, are required to define a GFEM. Assuming only L_\infty-coefficients we prove convergence of optimal order.

(C6 oral) **Exploiting local macroscopic quasi-homogeneities to accelerate multi-scale microstructure simulations**

J Gawad, M Khairullah, D Roose, A Van Bael

KU Leuven, Belgium

Multi-scale simulations in material modelling are computationally expensive if the fine-scale model must be evaluated at virtually every point in the macroscopic model. However, the macroscopic field variables primarily responsible for the evolution of fine-scale state variables often feature local quasi-homogeneities. In this paper we exploit this by making a verifiable assumption that the fine-scale state variables of similar RVEs, as well as the derived properties, subjected to similar macroscopic boundary conditions evolve along nearly identical trajectories. Adjacent points in the macroscopic model can be then clustered together in the regions of low variance in the macroscopic field responsible for evolution of the fine-scale model. In this work we follow this concept to improve a hierarchical multi-scale crystal plasticity framework based on the FEM. Technically, a number of adjacent integration points in the macroscopic FE mesh is be clustered together, so that they share the same fine-scale state variables and, as a consequence, they have identical material properties. The evolution of the fine-scale variables can be then computed just at the representative points of the clusters, provided the loading conditions of all the points belonging to any individual cluster are sufficiently similar. Optimal configurations of the clusters change in time, so an adaptive clustering strategy is followed. From a presented set of test cases we conclude that large performance gains (e.g. a speedup of 25) can be obtained at the expense of introducing only a minor (e.g. below 1%) modelling error.

(C7 invited) **Error estimators for first-principle molecular simulation**

E Cancès[1,3], G Dusson[2], Y Maday[2], B Stamm[2] and M Vohralik[3]

[1]CERMICS - Ecole des Ponts, France, [2]UPMC, USA, [3]INRIA Paris, France

First-principle molecular simulation based on electronic structure calculation has become an essential tool in chemistry, condensed matter physics, molecular biology, materials science, and nanosciences.

The difference between the exact value of a physical quantity (e.g. the lattice parameter of a perfect crystal, its phonon spectrum, the band gap of a semiconductor, the formation energy of a point defect, ...) and the value obtained by a simulation, can be decomposed in five components: the modeling error, the discretization error, the algorithmic error, the implementation error, and the calculation error. In this talk, I will explain how to define and analyze the various components of the error, and I will present recent results allowing one to accurately estimate the discretization and algorithmic errors for Kohn-Sham DFT models.

This is a first step toward the design of certified and optimized first-principle molecular simulation softwares, in which

- numerical simulation results are systematically complemented by guaranteed error bars ;
- the computational cost (CPU and memory requirement) is optimized by an adaptive choice of the model and of the numerical parameters (e.g. energy cut-off, number of k-points, convergence thresholds, ... for a Kohn-Sham calculation of a crystal in a planewave basis set).

(C7 oral) **Foundations of kinetic Monte Carlo models and the accelerated dynamics techniques**

T Lelievre

Ecole des Ponts ParisTech, France

I will present a mathematical framework to understand and justify kinetic Monte Carlo models and the harmonic transition state theory. This mathematical framework is based on the notion of quasi stationary distribution. Using this point of view, I will describe how accelerated dynamics techniques proposed by A.F. Voter in the late nineties can be understood and justified. In particular, we will present generalizations of the Parallel Replica method which widen its range of applicability.

[1] D. Aristoff, T. Lelièvre and G. Simpson, The parallel replica method for simulating long trajectories of Markov chains, AMRX, 2, 332-352, (2014)

[2] A. Binder, T. Lelièvre and G. Simpson, A Generalized Parallel Replica Dynamics, Journal of Computational Physics, 284, 595-616, (2015)

[3] C. Le Bris, T. Lelièvre, M. Luskin and D. Perez, A mathematical formalization of the parallel replica dynamics, Monte Carlo Methods and Applications, 18(2), 119-146, (2012)

[4] T. Lelièvre, Accelerated dynamics: Mathematical foundations and algorithmic improvements, Eur. Phys. J. Special Topics 224, 2429-2444, (2015)

(C7 oral) **Stochastic processes and diffusive molecular dynamics**

G Simpson[1], B Farmer[2], M Luskin[2], P Plechac[3] and D Srolovitz[4]

[1]Drexel University, USA, [2]University of Minnesota, USA, [3]University of Delaware, USA, [4]University of Pennsylvania, USA

Diffusive Molecular Dynamics (DMD) is a novel approach to problems in molecular dynamics that aims to reach the diffusive time scale of milliseconds and beyond. To accomplish this, DMD "averages out" the vibrational time scale of femtoseconds and evolves probability densities at atomistic sites. This requires the approximation of a probability distribution in an extended state space by a synthetic approximate distribution, which can easily be sampled. The mean occupancy at the atomic sites are then evolved according to a system of coupled ODEs, under a so-called Master Equation, but no underlying stochastic process is given in the current formulation. In this work, we propose and examine a stochastic process which gives rise to similar dynamics as DMD. This primitive model also offers a way to connect DMD to a more traditional MD models.

(C7 oral) **Assessment of phase-field-crystal concepts using long-time molecular dynamics**

W A Curtin and K Baker

École Polytechnique Fédérale de Lausanne, Switzerland

The ability of the phase-field-crystal (PFC) model to quantitatively predict atomistic defect structures in crystalline solids is addressed [1]. First, theoretical aspects of the PFC model are discussed in the context of obtaining quantitative results in crystals. A specific example illustrates major points. Specifically, accelerated MD is used to compute the one-particle probability density $\rho 1(r)$ in a complex atomistic defect consisting of a Lomer dislocation with an equilibrium distribution of vacancies, and the results are considered within the framework of PFC. As expected, $\rho 1(r)$ shows numerous spatially localized peaks with integrated densities smaller than unity, as arise in PFC. However, $\rho 1(r)$ actually corresponds to a time-averaged superposition of a few well-defined atomic configurations each with well-defined energy. The deconvolution of $\rho 1(r)$ to obtain these distinct configurations is infeasible. Using a potential energy functional that accurately computes the energies of distinct configurations, the potential energy computed using $\rho 1(r)$ differs from the actual atomistic energy by $\sim$50 eV (divided among $\tilde{}$46 core atoms). Introducing correlations can not significantly reduce this error. The simulations further show that energy barriers between configurations varying by up to 0.5 eV, so the simple kinetic law in PFC cannot capture the true time evolution. Overall, these results demonstrate, in one non-trivial case, that the PFC model is probably unable to predict atomistic defect structures, energies, or kinetic barriers, at the quantitative levels needed for application to problems in materials science.

[1] K. L. Baker and W. A. Curtin, Physical Review B 91, 014103 (2015)

(C7 oral) **Predicting solute segregation kinetics and properties in binary alloys from a dynamical variational gaussian model**

C Sinclair, J Rottler and E Dontsova

University of British Columbia, Canada

The thermodynamics and kinetics of solute segregation in crystals is important for controlling microstructure and properties. Prime examples are the effects of solute drag on interface migration and of static strain aging on the yield stress. A fully quantitative prediction of solute segregation is difficult, however, due to the spatially varying solute-defect binding energies that are atomic in origin. Moreover, as solute segregation enhances (locally) the solute concentration, dilute approximations for the underlying thermodynamics and kinetics become questionable.

We present a dynamical version of the variational gaussian method for binary alloys [1] and illustrate its potential for select problems involving solute segregation including static strain aging in Al-Mg alloys [2]. Our model adapts the recently proposed Diffusive Molecular Dynamics (DMD) model for vacancy diffusion in crystals where a phonon-free description of solids is coupled with statistical averaging over various configurations to allow for the efficient calculation of free energies. In the alloy version of the model, the free energy is minimized by optimizing the atomic positions and vibrational amplitudes while relaxational dynamics are used to evolve the solute concentration field based on the local energy landscape. We show that this model successfully describes solute redistribution over diffusive timescales. In contrast to traditional continuum diffusion treatments, atomistic effects are automatically accounted for, and full kinetic pathways of the evolution of material properties are revealed in addition to the equilibrium properties.

[1] E. Dontsova, J. Rottler, C. W. Sinclair, Phys. Rev. B 90, 174102 (2014)
[2] E. Dontsova, J. Rottler, C. W. Sinclair, Phys. Rev. B 91, 224103 (2015)

(C8 invited) **Multiscale computations with MsFEM: a posteriori error estimation, adaptive strategy, and coupling with PGD model reduction**

L Chamoin[1] and F Legoll[2]

[1]ENS Cachan INRIA, France, [2]Ecole des Ponts ParisTech, France

The Multiscale Finite Element Method (MsFEM) is a powerful numerical method in the context of multiscale analysis. It uses basis functions which encode details of the fine scale description, and performs in a two-stage procedure: (i) offline stage in which basis functions are computed solving local fine scale problems; (ii) online stage in which a cheap Galerkin approximation problem is solved using a coarse mesh. However, as in other numerical methods, a crucial issue is to certify that a prescribed accuracy is obtained for the numerical solution. In the present work, we propose an a posteriori error estimate for MsFEM using the concept of Constitutive Relation Error (CRE) based on dual analysis. It enables to effectively address global or goal-oriented error estimation, to assess the various error sources, and to drive robust adaptive algorithms. We also investigate the additional use of model reduction inside the MsFEM strategy in order to further decrease numerical costs. We particularly focus on the use of the Proper Generalized Decomposition (PGD) for the computation of multiscale basis functions. PGD is a suitable tool that enables to explicitly take into account variations in geometry, material coefficients, or boundary conditions. In many configurations, it can thus be efficiently employed to solve with low computing cost the various local fine-scale problems associated with MsFEM. In addition to showing performances of the coupling between PGD and MsFEM, we introduce dedicated estimates on PGD model reduction error, and use these to certify the quality of the overall MsFEM solution.

(C8 oral) **Localized adaptive model reduction for multi-scale problems**

F Schindler and M Ohlberger

University of Muenster, Germany

We present recent advances in the context of the localized reduced basis multi-scale method (LRBMS) for parametric elliptic multi-scale problems with possibly heterogeneous diffusion coefficient (see [1,2]). The numerical treatment of such parametric multi-scale problems is characterized by a high computational complexity, arising from the multi-scale character of the underlying differential equation and the additional parameter dependence.

The LRBMS method can be seen as a combination of numerical multi-scale methods and model reduction using reduced basis methods to efficiently reduce the computational complexity with respect to the multi-scale as well as the parametric aspect of the problem, simultaneously. The LRBMS is equipped with a localized a posteriori error estimate based on conservative flux reconstruction which provides an efficient and rigorous bound on the full approximation error with respect to the weak solution.

We present recent advances of the online adaptive LRBMS (which is based on this localized error estimate) together with experiments to demonstrate the applicability of the resulting algorithm to single phase flow in heterogeneous media.

[1] Ohlberber, M. ; Schindler, F.: *Error control for the localized reduced basis multi-scale method with adaptive on-line enrichment.* SIAM J. Sci. Comput., 37(6):A2865A2895, 2015.

[2] F. Albrecht, B. Haasdonk, S. Kaulmann, and M. Ohlberger, *The localized reduced basis multiscale method*, in Proceedings of Algoritmy 2012, onference on Scientific Computing, Vysoke Tatry, Podbanske, 2012, Slovak University of Technology, Bratislava, 2012, pp. 393-403.

(C8 oral) **Numerical upscaling by a localized orthogonal decomposition**

P Henning[1], A Målqvist[2] and D Peterseim[3]

[1]KTH Royal Institute of Technology, Sweden, [2]Chalmers University of Technology, Sweden, [3]University of Bonn, Germany

In this talk, we give an introduction to the concept of the Localized Orthogonal Decomposition (LOD), which is a multiscale method that does not rely on assumptions of scale separation or regularity. The central idea of the LOD is to construct an optimal low dimensional generalized finite element space that incorporates the variations of data functions in a natural way. The multiscale space is constructed by finding the orthogonal complement of the kernel of an interpolation operator with respect to a problem specific scalar product. The operator maps into a classical 'coarse' finite element space. We present a general convergence result for this approach and show numerical experiments on problems with high contrast and conductivity channels.

(C8 oral) **An embedded corrector problem for stochastic homogenization**

V Ehrlacher[1], E Cancès[2], F Legoll[2] and B Stamm[3]

[1]CERMICS, Ecole des Ponts Paristech & INRIA, France, [2]Ecole des Ponts Paristech & INRIA, France, [3]Pierre-and-Marie-Curie University, France

A very efficient algorithm has recently been introduced in [1] in order to approximate the solution of implicit solvation models for molecules. The main ingredient of this algorithm relies in the clever use of a boundary integral formulation of the problem to solve. The aim of this talk is to present how such an algorithm can be adapted in order to compute efficiently effective coefficients in stochastic homogenization for random media with spherical inclusions. To this aim, the definition of new approximate corrector problems and approximate effective coefficients is needed and convergence results in the spirit of [2] are proved for this new formulation. Some numerical test cases will illustrate the behaviour of this method.

[1] "Domain decomposition for implicit solvation models", Eric Cancès, Yvon Maday, Benjamin Stamm, The Journal of Chemical Physics 139 (2013) 054111

[2] "Approximations of effective coefficients in stochastic homogenization", Alain Bourgeat, Andrey Piatnitski, Annales de l'institut Henri Poincaré (B) Probabilités et Statistiques 40 (2004) page 153-165

(C9 invited) **Speculatively parallel temperature accelerated dynamics**

A Voter

Los Alamos National Laboratory, USA

Temperature accelerated dynamics (TAD) is a powerful atomistic approach for reaching long time scales for systems whose dynamics are characterized by activated processes, especially when the energy barriers are high. In TAD, a basin-confined simulation at a high temperature is employed to discover attempted escape events in a way that allows the assignment of a time t_low (approximate, but controllably accurate) for the same event occurring in a hypothetical trajectory at the lower, proper temperature. High- and low-temperature escape times typically will not occur in the same order, as high-barrier processes are sped up more by the increase in temperature. After the basin-confined, high-temperature trajectory has reached a certain total time (t_stop), one can say with a specified confidence that the first escape event at low temperature has been observed. The system is then moved to the new state corresponding to this event, the clock is advanced by t_low for this event, and the TAD procedure is begun again in the new state.

In this talk, I will describe a novel approach for parallelizing TAD: speculatively parallelized TAD (SpecTAD) [1]. In SpecTAD, we spawn a child process in parallel each time an attempted escape event is observed, if it has a chance of becoming the accepted event. This child process, which corresponds to a complete, independent TAD simulation in the state to which the system made its attempted escape, is continued until and unless it becomes clear that this event is not the one that will be accepted by the parent TAD simulation. SpecTAD gives a significant additional speedup over conventional TAD when t_stop is much longer than the time at which the ultimately accepted event is first attempted. A SpecTAD trajectory can advance from state to state as rapidly as the (correct) transitions occur at high temperature. Moreover, this approach can be combined efficiently with parallel replica dynamics to accumulate the high-temperature time more quickly. I will describe the SpecTAD method, give examples of its application, and discuss situations where its ability to eliminate the waiting time until t_stop introduces new possibilities for simulations that would be unfeasible with conventional TAD.

[1] R.J. Zamora, B.P. Uberuaga, D. Perez, and A.F. Voter, The modern temperature-accelerated dynamics approach. The Annual Review of Chemical and Biomolecular Engineering 7, 3.1-3.24 (2016)

(C9 oral) **Coupled atomistic/discrete-dislocation method in 3d**

M Hodapp, W Curtin, J-F Molinari and G Anciaux

Ecole Polytechnique Fédérale de Lausanne, Switzerland

Atomistic modelling is a valuable tool for material science applications on the nanoscale but becomes impractical with increasing simulation size due to the high computational cost. Realistic engineering applications require model reduction/coarse-graining approaches which partially overcome this problem by exploiting the elastic response of uniform crystals under homogeneous deformation far from defects of interest. Problems in micro-plasticity involve a large number of dislocations moving over long distances, making full atomistic resolution prohibitive. To address this bottleneck, we extend the Coupled Atomistic and Discrete Dislocations (CADD) method [1] to three dimensions. This is accomplished by a domain-decomposition approach with mechanical coupling through elasticity and the transition of a dislocation between atomistic and continuum-line representations through a “template” imposed at the atomistic/continuum interface in the vicinity of dislocation cores that enriches the continuum-line description. A dislocation detection algorithm inside the atomistic region serves as a Dirichlet-type boundary condition on the discrete dislocations. The coupled problem possesses severe challenges due to the highly non-symmetric and heterogeneous interface structure. To solve the problem numerically we cast it into an alternating Schwarz-type framework which circumvents the concurrent coupling while preserving necessary computational gains. The domain-specific calculations are performed using open-source codes (LAMMPS and ParaDis) within the LibMultiscale framework (lsms.epfl.ch).

As a reference problem we study a bow-out of a dislocation in a semi-periodic box, in which parts are described atomistically and by the continuum model, respectively. A fully atomistic model is used to validate the coupled method.

[1] L. Shilkrot et al., JMPS 52, 2004

(C9 oral) **Using embedding into a polarizable solid to study defects in insulators**

A Shluger and D Gao

University College London, UK

An embedded cluster method is a self-consistent version of QM/MM method developed for calculating properties of defects in ionic solids. It is most useful for modelling defects in amorphous materials, at rough surfaces and grain boundaries, where using periodic boundary conditions is often unfeasible. The important part of the system treated quantum mechanically (QM) is embedded in the rest of the system, treated classically, using embedding pseudopotentials at the interface between the two regions. The classical subsystem is treated using a polarisable ion model and responds self-consistently to the changes in the structure and charge distribution in the QM subsystem. We will describe methods for developing embedding potentials in different systems and their implementations in GUESS and CP2K codes and will give examples of applications. These include the calculations of defect properties in amorphous SiO_2, at surfaces and grain boundaries in MgO, and adsorption of organic molecules at surfaces of alkali halides. We will discuss the limitations of this method and challenges for constructing embedding potentials for more complex semi-covalent oxides.

(C9 oral) **A study of conditions for dislocation nucleation in coarser-than-atomistic scale models**

A Garg[1], A Acharya[2] and C Maloney[3]

[1]FM Global, USA, [2]Carnegie Mellon University, USA, [3]Northeastern University, USA

We perform atomistic simulations of dislocation nucleation in defect free crystals in 2 and 3 dimensions during indentation with circular (2D) or spherical (3D) indenters. The kinematic structure of the theory of Field Dislocation Mechanics (FDM) is shown to allow the identification of a local feature of the atomistic velocity field in these simulations as indicative of dislocation nucleation. It predicts the precise location of the incipient spatially distributed dislocation field, as shown for the cases of the Embedded Atom Method potential for Al and the Lennard–Jones pair potential. We demonstrate the accuracy of this analysis for two crystallographic orientations in 2D and one in 3D. Apart from the accuracy in predicting the location of dislocation nucleation, the FDM based analysis also demonstrates superior performance than existing nucleation criteria in not persisting in time beyond the nucleation event, as well as differentiating between phase boundary/shear band and dislocation nucleation. Our analysis is meant to facilitate the modelling of dislocation nucleation in coarser-than-atomistic scale models of the mechanics of materials.

(C9 oral) **Using Zwanzig's technique to investigate stochastic defect motion over small and large barriers**

T Swinburne and S Dudarev

Culham Centre for Fusion Energy, UK

The rate at which a defect responds to deterministic forces (from internal and external stresses, migration barriers, chemical bonding etc.) is typically controlled by thermal stochastic forces, whose cumulative action gives rise to viscous drag, thermally activated barrier crossing and diffusive transport.

In this work, we use Zwanzig's technique to derive a generalized Langevin equation for a crystal defect, starting from the 3N-dimensional equation of motion of the host crystal. Our approach produces a method to extract a well-defined total force on a crystal defect or dislocation directly from the atomic forces, which can be evaluated in static or dynamic atomistic simulations. We show that dynamical force averages have attractive convergence properties compared to velocity or position averages, due to their weaker coherence, whilst in appropriate limits the determinisic component of the defect force reduces to the Peach-Koehler force and can perfectly reproduce any migration barriers.

With only mild assumptions on the underlying thermal vibrations, we derive an analytical expression for the defect-vibrational coupling, allowing us to analytically investigate Kramers' rate theory, which solves the Fokker-Planck equation to give a crossing rate valid for arbitrarily small or large barriers. Our results resolve a puzzling failure of phonon scattering theories and offer new insights into the correspondence between Vineyard's and Kramers' transition state theories.

[1] TD Swinburne and SL Dudarev, Phys. Rev. B 92, 134302 (2015)
[2] TD Swinburne, SL Dudarev and AP Sutton, Phys. Rev. Lett. 113, 215501 (2014)

(C10 invited) **Adaptive GMsFEM and its applications**

E Chung[1] and Y Efendiev[2]

[1]The Chinese University of Hong Kong, Hong Kong, [2]Texas A&M University, USA

In this talk, we present the adaptive generalized multiscale finite element method (GMsFEM) and its applications. The method is a generalization of the classical multiscale finite element method, and allows basis enrichments. The basis functions are constructed from some snapshot spaces and some dimensional reduction procedure. In addition, some local residual based error indicators are developed and guide how basis functions are included. We will also discuss the online basis functions, where new basis functions are computed in the online stage. We will present some theories and numerical examples. This research work is partially supported by the Hong Kong RGC General Research Fund (Project: 400813).

(C10 oral) **Analysis and numerical simulation of patterns in incommensurate 2D layered materials**

P Cazeaux and M Luskin

University of Minnesota, USA

Recent experimental discovery of numerous 2D materials, such as graphene or boron nitride, opened many exciting perspectives including the possibility of stacking a few layers of such materials.

One of the main issues towards numerically exploring the possibilities of this atomic-scale Lego game is the generic incommensurate character of heterostructures. Indeed, the difference between cristal-line structure of the individual layers, or the rotation of one layer relative to another, in general destroys the periodic character of the system while sometimes producing a mesoscale Moire pattern or a super-lattice.

In this presentation, we will discuss experimentally observed patterns created by mechanical relaxation of slightly twisted 2D layers. We will show how these patterns result from commensurate-incommensurate transitions predicted by rigorous analysis of Frenkel-Kontorova-like models and Aubry-Mather theory. We will present and analyse numerical multiscale methods adapted to these weakly-coupled layers, and discuss some numerical simulations.

(C10 oral) **Multiscale finite element type approaches for convection-dominated problems in heterogeneous media**

F Legoll

Ecole des Ponts and INRIA, France

Advection-diffusion equations arise in many engineering applications, and it is often the case that convection dominates over diffusion. In that regime, standard numerical approaches (such as P1 Finite Element approximations) provide approximations of poor accuracy, and stabilized methods (in the spirit of SUPG) are required.

In this work, we consider the case when the problem is multiscale, in addition to being convection-dominated. Groundwater pollution through infiltration of a fluid in porous media is one example of such problems. Numerical homogenization techniques, such as MsFEM-type approaches, are in order to handle the presence of several scales.

We show here how to adapt the stabilized methods and the MsFEM-like multiscale methods to efficiently solve multiscale advection-diffusion problems in the convection-dominated regime. Different possibilities to simultaneously treat both difficulties will be described and compared.

[1] C. Le Bris, F. Legoll and F. Madiot, A numerical comparison of some Multiscale Finite Element approaches for convection-dominated problems in heterogeneous media, arXiv preprint 1511.08453

(C10 oral) **Long-range electrostatic energies and forces for fragmentation methods**

F Heber

Universität des Saarlandes, Germany

Fragmentation methods are an ideal ansatz for creating multi-scale methods from the ab-initio level. They take a molecular system and split it up into small fragments. Energy and force calculations are performed on these fragments only and the resulting values are cleverly summed up in a related way. If the number of fragments is limited to increasing only linearly with the number of atoms, a linear-scaling electronic structure method naturally results. The fragments form a good basis for coarse-graining or fitting of empirical potentials.

However, because of the limited scope of the molecular fragments, neither static nor dynamic long-range interactions are taken fully into account.

In [1] all of the well-known methods for linear-scaling computations of Coulomb interactions are reviewed. such as FMM, P^3M, PME, hierachical methods, and multi-grid methods.

We propose that multi-grid methods can be readily used to incorporate calculation of long-range electrostatic energies and forces into fragmentation methods. The central idea is to take the electronic and nuclei charge distributions and perform the same summation procedure on these charge distribution as is done on the energies and forces. From the resulting charge distributions Coulomb potentials can be obtained via the linear-scaling multi-grid method and then long-range energies and forces calculated.

We show examples of electronic structure calculations with this fragmentation method and the versatile multigrid solver including long-range interactions and discuss possible obstacles and how to overcome them.

[1] Godehard Sutmann et al.. Comparison of scalable fast methods for long-range interactions. Physical Review E, 88(6):063308, Dec 2013

(C10 oral) **From atoms to models of aging in metal tritides**

P Schultz and C Snow

Sandia National Laboratories, USA

Predictive modelling of aging in metal tritides-tritium decay, helium migration, bubble nucleation and growth, and eventual materials rupture-requires detailed knowledge of the microscopic processes and mechanical properties of the tritide material. Challenges in sample generation and interpretation of experiments makes obtaining this data, and assessing its reliability, difficult or impossible. Density functional theory calculations model mechanical properties of metals with high precision, and can generate very accurate data for input to mesoscale models—or can they? We illustrate the important role that careful consideration of uncertainties and validation play in any useful upscaling analysis. Detailed attention to the numerical aspects of the DFT modelling is shown to lead to significant uncertainties into the assessment of mechanical properties of the rare earth dihydrides. Aggregate uncertainties in the DFT simulations and upscaling into bubble growth and fracture model parameters can be rather large. Interplay with experimental data allows meaningful validation and quantifiably reliable estimates of parameters needed for mesoscale models of bubble growth and fracture. In addition, this analysis provides interesting and credible insights into the phase changes between the cubic and tetragonal hydride phases exhibited by lanthanide and early transition metal hydrides.

(C11 invited) **Reversal-time scaling in low-damping ferromagnetic models**

K Newhall

UNC Chapel Hill, USA

A large variety of observable phenomena, such as magnetization reversals, are mathematically described as transitions between metastable states in a system with many degrees of freedom. These transition times are often exponential in an energy barrier height and an inverse temperature. In a one-dimensional system, I show how time-scale separation between energy and precessional dynamics can be exploited to compute thermally assisted transition times, including a damping-dependent prefactor of the exponential term. I then show how this type of damping-dependent scaling only remains in higher or infinite dimensional systems when there is a reduced, effectively one dimensional system, that captures the dynamics.

(C11 oral) **Atomistic/continuum modelling of magnetisation dynamics of ferromagnetic materials**

M Poluektov, G Kreiss and O Eriksson

Uppsala University, Sweden

Physical properties of materials are often highly dependent on the underlying microstructure and affected by presence of defects and/or heterogeneities at the atomistic length scale. Multiscale atomistic-continuum models allow investigating the influence of the small-scale phenomena on macroscopic quantities without using the fine-scale resolution over the entire computational domain.

The dynamic behaviour of ferromagnetic materials can be simulated either at the atomistic scale, where spin magnetic moments of individual atoms are considered while atomic positions are fixed, or at the continuum scale, where the evolution of coarse-grained quantities, such as volume-averaged magnetisation, is described by the specific PDEs. Interfacing these descriptions by domain partitioning, which implies the existence of an explicit interface between atomistic and continuum regions, leads to some computational difficulties, such as the mismatch between non-local atomistic interactions and local continuum description and, in the case of dynamics, high frequency wave reflections at the interface due to change in discretisation.

In this talk, the technique of introduction of numerically-damped quasi-non-local atoms at the proximity of the interface, which interact differently with the atomistic and continuum regions and which absorb high frequency waves, is discussed. To illustrate the applicability of the developed method, examples of a propagation of spin-waves and a motion of domain walls in ferromagnetic materials with crystallographic defects are shown.

(C11 oral) **Stochastic approach to cluster dynamics method**

P Terrier[1], G Stoltz[2], M Athènes[3], T Jourdan[3]and G Adjanor[4]

[1]Université Paris-Est, CERMICS (ENPC) & CEA, DEN/SRMP, France, [2]CEA, DEN/SRMP, France, [3]EDF, R&D, France

Aging in irradiated materials requires the treatment of defect cluster evolution, from the nucleation of small and unstable small size clusters to the growth of more stable large size clusters. Cluster dynamics method has been successfully used to study such a phenomenon. It is a system of ODEs describing the number of clusters of various sizes. However, it becomes computationally prohibitive when large clusters appear. In order to reduce the numerical complexity of the model, we develop a coupling approach between the ODE and a limiting model obtained in the asymptotic regime of large cluster sizes. We rigorously derive the limiting PDE by a rescaling procedure, and propose a stochastic approach to solve this equation. The coupling method then allows to simultaneously evolve the master equation (for small size clusters) and the PDE part.

(C11 oral) **A numerical study of non-linear polycrystalline materials through a homogenization technique**

T M Schlittler and R Cottereau

Laboratoire MSSMat – CentraleSupelec, France

In this talk, we will focus on the study of polycrystalline materials, such as most metals and many types of ceramics, using numeric multi-model coupling methods. Different scales and models are associated to these materials, and here we are interested in two of them: a micro scale, where a heterogeneous elasto-plastic model is considered, and a macro scale, with a homogeneous non-linear model.

The motivation of this work is to identify the properties of the macro scale model knowing those of the micro scale model. From the numerical point of view, one can perform a homogenization on the multi-scale system. Such methods are very sensitive to the boundary conditions and to the ratio between the characteristic scales of the models, and can introduce a bias to the resulting homogenized macro scale tensor if this ratio is too high. In the cases where a stochastic model is used to represent the micro scale, this bias is still present even after using an infinite number of Monte-Carlo realizations.

We will present an application of a homogenization which reduces this bias, based on the Arlequin method applied to a polycrystalline material. We will model the micro scale system using a stochastic, non-linear micro scale model and a homogeneous macro scale model, and the results obtained will be compare with those of the literature.

This work benefited from French state funding managed by the National Research Agency under project number ANR-14-CE07-0007 CouESt.

(P1.11) **Quantum molecular dynamics: accelerating diffusion via parallel replica method**

I Novoselov and A Yanilkin

All-Russian Research Institute of Automatics, Russia

Typically, time of quantum molecular dynamic simulation does not exceed several tens of picoseconds, while vast range of technologically important and scientifically interesting processes take place over longer times. Diffusion is a good example of the latter. The standard way of calculating diffusion properties is a classical molecular dynamic simulation accelerated by parallel replica dynamics (PRD) [1]. Accuracy of this approach is limited by precision of classical interatomic potential used and the error introduced by PRD technique.

In this work we propose a method of reducing both of the uncertainties. Firstly, we implemented PRD coupled with DFT code, thus we avoid the usage of empiric classical potentials and improve precision of describing interatomic interactions. We also perform detailed analysis of the influence of PRD's internal parameters on its outcome. This allows us to estimate and minimize the error introduced by the usage of the acceleration technique.
We tested our approach for the case of self-diffusion in aluminum. Finally, we employed the method to calculate diffusion coefficient of hydrogen in titanium hydride. Obtained values demonstrate much better agreement with experimental data than the results of classical molecular dynamic simulations.

[1] A.F. Voter, Phys. Rev. B. 1998, 57(22): 985 - 988

(P1.12) **Influence of meso and nanoscale structure on the properties of highly efficient small molecule solar cells**

P Friederich[1], T Mönch[2], F Holzmueller[2], B Rutkowski[3], J Benduhn[2], T Strunk[4], C Körner[2], K Vandewal[2], A Czyrska-Filemonowicz[3], W Wenzel[1] and K Leo[2]

[1]Karlsruhe Institute of Technology, Germany, [2]TU Dresden, Germany, [3]AGH University of Science and Technology, Poland, [4]Nanomatch GmbH, Germany

The nanoscale morphology of the bulk heterojunction absorber layer in an organic solar cell (OSC) is of key importance for its efficiency. The morphology of high performance vacuum-processed, small molecule OSCs based on oligothiophene derivatives (DCV5T-Me) blended with C_{60} on various length scales is studied. We combine meso and nanoscale simulations with experimental results to gain unique insights into the relation between processing, morphology, and efficiency of the final devices. Mesoscopic Monte Carlo simulations are used for coarse grained simulations of the bulk heterojunction morphology. The findings are combined with density functional theory calculations to model the electronic structure and charge transport properties. It is shown that the connectivity of the oligothiophene-C_{60} network is independent of the material domain size. The decisive quantity controlling the internal quantum efficiency is the energetic disorder induced by material mixing, strongly limiting charge and exciton transport in the OSCs.

(P1.13) **Facilitating reproducibility of multi-scale simulations using a modular workflow system**

T Strunk[1], T Neumann[2], P Friederich[2] and W Wenzel[2]

[1]Nanomatch GmbH, Germany, [2]Karlsruhe Institute of Technology, Germany

Simulations on multiple scales involve several different steps, each developed by an expert in his precise field. One such example is the calculation of electronic properties of organic thin-films, which requires the accurate calculation of microscopic single molecule properties, the generation and characterization of the entire morphology and ultimately the calculation of electronic properties on an extended macroscopic thin-film using QM technologies. Even the reproduction of one such multi-scale simulation from start to finish often requires knowledge of each individual step making it impossible to immediately use a multi-scale tool as a scientific user new to the toolkit. Here we show a workflow environment, which embeds each step in a testable and modular fashion and saves it in a workflow to reproducibly execute a multi-scale simulation from start to finish.

While previously both expert developers and scientific users were exposed to the same configuration language, developers can integrate their program tackling a problem on a specific scale using a rapid prototyping GUI language and only expose options required at runtime. Using a flexible script based system these modules can then be linked to exchange data and are run on a UNICORE-based architecture independent of the used HPC resources. We hope that this workflow environment will help ease reproducibility of scientific discoveries and further allow the commercialization of existing multi-scale toolkits into large-scale material screening applications.

(P1.14) **Feasible and reliable AB initio calculation of f-elements-bearing materials relevant for nuclear waste management**

P Kowalski, G Beridze, Y Li, B Xiao and E Alekseev

Forschungszentrum Juelich, Germany

Safe management of nuclear waste is a serious problem faced by the nuclear technology utilizing countries. Significant research effort is thus devoted to the development of methods that could be used for conditioning of long-lived actinides and their safe disposal in a deep geological rock formation. We contribute to such research with the atomistic simulations by providing a unique, atomic-scale insight on the radionucline-involving processes that determine the materials properties, which are often inaccessible to the experimental techniques. However, first principle atomistic simulations of radionuclide-bearing materials are not straightforward. This is because Density Functional Theory (DFT) - the only method of choice for *ab initio* simulations of complex fluids and solids - often fails for materials containing strongly correlated *f*-electrons and higher order methods (e.g. hybrid functionals, CCSD(T)) are unfeasible for time-efficient simulations of these systems. Searching for a feasible and reliable computational method we found that DFT+*U* method with the Hubbard *U* parameter derived ab initio for each *f*-element in its oxidation state and local bonding structure, and with the properly chosen exchange-correlation functional, results in a very good predictions of the structural and thermodynamic properties of various actinide- and lanthanide- bearing materials such as uranium- and thorium-bearing compounds and solids, and monazite ($LnPO_4$)- and pyrochlore ($Ln_2(Zr,Hf)_2O_7$)-type ceramics, for which DFT often fails. We thus demonstrate that with this method one can reliably simulate the properties of even chemically complex and experimentally challenging actinide-bearing materials.

(P1.15) **Representing atomic systems**

J Bulin and J Hamaekers

Fraunhofer Institute for Algorithms and Scientific Computing SCAI, Germany

In a lot of important simulation methods, atomic systems are represented by the cartesian coordinates of their atoms. While this representation is well suited for applications like molecular dynamics, it may cause problems when invariance under rotations, translations or permutations is desirable. This occurs frequently when potential energies are involved, for example when learning potential energy surfaces via machine learning.

We will review state-of-the-art representations of molecules and periodic crystals. This also includes an overview over techniques that are used to calculate similarity measures for particle systems. Finally we present ideas how these representations can be used to setup a database that contains a large number of atomic systems. The challenge here is to do it in such a way that it is possible to find rotated, permuted or translated instances of a given reference system in the database.

(P1.16) **A hybrid parallel numerical algorithm for three-dimensional phase field modeling of crystal growth**

P Strachota and M Beneš

FJFI CVUT v Praze, Czech Republic

We introduce a hybrid parallel numerical algorithm for solving the phase field formulation of the anisotropic crystal growth during solidification. The implementation is based on a finite volume discretization scheme and uses the MPI and OpenMP standards. The algorithm has undergone a number of efficiency measurements and parallel profiling scenarios. We compare the results for several variants of the algorithm and decide on the most efficient solution. Furthermore, we assess the advantages of hybrid parallelization on current high performance computing clusters.

(P1.17) **Numerical and theoretical modelling of freeze-thaw damage in concrete**

T Zhou[1], E Masoero[2], R Pellenq[3] and M Bazant[1]

[1]Massachusetts Institute of Technology, USA, [2]Newcastle University, UK, [3]CNRS, France

Ionic correlation forces are known to be an origin of charged particle attraction in colloidal materials. However this mechanism remains poorly understood. Most previous work on this topic focus on only 1 type of cations in the pore solution, while in realistic situations there are multiple species of ions with different valence of charge. In this work we present numerical simulation and theoretical analysis of porous media with multiple species of ions in the pore solution. This effect is most boosted during fluid-solid phase transition of the pore solution, e.g., in freeze-thaw cycles of concrete, since the ion concentrations are enhanced in the remnant fluid between the pore substrate and the solid phase, as well as the smaller pores which remains fluid at relatively low temperature. We first present the model with only monovalent/divalent ions, compared to known results. Then we present a novol model with a mixture of ions of different valences.

(P1.18) **Development of EAM Fe-Y interaction potential**

S Koch, P Vladimirov and A Möslang

Karlsruhe Institute of Technology, Germany

Empirical Fe-Y-O interaction potentials are required for description of oxide particles nucleation and growth, modelling of dislocation interaction with oxide particle as well as for simulation of various phenomena occurring at the oxide-matrix interface under irradiation in ODS steels.

As an intermediate step, an interaction potential for Fe-Y system based on the embedded atom method (EAM) is being developed in this work. Up to now two elemental EAM Potentials were readily adopted, for bcc Fe and hcp Y, which are suitable for a development of the Fe-Y alloy potentials. The parameters were successfully determined by computing the lattice constant, cohesion energy, elastic constants and various vacancy formation energies as well as self-interstitial formation energies analytically. For obtaining better alloy parameter sets the following vacancy formation energies were reproduced more accurately: In bcc Fe, single vacancy formation energy 1.75 eV, di-vacancy formation energy 3.35 eV, 3.37 eV and 3.65 eV as 1st Nearest Neighbour (NN), 2nd NN and 3rd NN, respectively. In hcp Y: single vacancy formation energy 1.62 eV.

These two components were then used to build a Fe-Y alloy potential. Different parameter sets were investigated and the best one was chosen by comparisons to the Rose equation and universal fitting relations.

Modelling several Fe-Y phases, like Fe2Y and Fe17-Y2,w.r.t. lattice constants and cohesion energies is still in process. The resulting Fe-Y potential could be extended by Fe-O and Y-O, resulting in the Fe-Y-O interaction potential which might be further improved by extension to modified embedded atom method (MEAM).

(P2.10) **A validated cellular-automata model for normal and abnormal grain coarsening using local transition functions with optimal cell connectivity**

D Aflyatunova and M Mahfouf

University of Sheffield, UK

Grain growth in metals strongly influences the microstructure and final properties, but it is difficult to study via experimental and statistical methods alone. Cellular Automata (CA) technique was successfully applied in [1] for modelling normal and abnormal grain growth using local transition functions, which required the counting of probabilities for a state-change (assigned a number that corresponds to the orientation angle) for each cell on the grid and the synchronous update of all lattice. However, a cell can only be transformed into another cell from the group of cells which are connected to the core cell via faces, and does not consider other surrounding cells in the suggested model. This limitation is circumvented in the present work when both groups of cells were considered, but with different priorities in order to reflect the influence of the lattice structure. The result is a new improved CA-based model which is generalised for both normal and abnormal grain coarsening and whose validation with experimental data showed a significant improvement in predictions in comparison with the original model. Furthermore, the new model structure also included grain boundaries that are more clear-cut in the same grain area, with a noticeable decreased roughness.

[1] Ye. Vertyagina, M. Mahfouf, and X. Xu., Journal of Materials Science, 48(16): 5517- 5527, August 2013.

(P2.11) **Ab initio trained neural-network driven kinetic Monte Carlo simulations of microstructure evolution of irradiated iron alloys**

L Messina[1], N Castin[2], C Domain[3] and P Olsson[4]

[1]CEA Saclay, France, [2]SCK-CEN, Belgium, [3]EDF R&D, France, [4]KTH Royal Institute of Technology, Sweden

Ferritic alloys are widely used as structural materials in nuclear power plants. The interaction of radiation-induced defects with impurities leads to a chemical rearrangement and often to a deterioration of the alloy mechanical properties. Such interaction represents a key component in modelling the microstructure evolution, essential for developing a predictive tool that can assess the alloy radiation response. Kinetic Monte Carlo methods are widely employed, but a common drawback is the impossibility of obtaining an accurate parameterization of all possible transition rates in multicomponent alloys, due to the high amount of possible atomic configurations of the local crystal environment.

To overcome this issue, neural networks have been recently introduced [1] as advanced interpolation schemes for the prediction of transition rates, trained on large databases of pre-calculated rates. The latter were obtained with molecular dynamic simulations based on an interatomic potential. However, the development of dedicated interatomic potentials is a difficult task and can be limited in reproducing the multifold properties of the alloy.

In this work, we investigate the possibility of training neural networks on transition-rate databases obtained with accurate density functional theory calculations, by simulating the microstructure evolution of thermally aged FeCu alloys. Though computationally costly, this approach will allow for a flexible extension of neural networks to alloys of varying chemical complexity and composition, with little added computational effort, and will open to more reliable predictive tools for the microstructure evolution of alloys exposed to extreme irradiation conditions.

[1] N.Castin et al., *J. Chem. Phys.* 135, 064502 (2011).

(P2.12) **An analytical investigation of Stress Assisted Grain Boundary Oxidation (SAGBO)**

L Cimbaro[1], A P Sutton FRS[1], D S Balint[1] and A T Paxton[2]

[1]Imperial College London, UK, [2]King's College London, UK

SAGBO is one of the most important mechanisms of time dependent intergranular cracking of nickel-based superalloys at high temperatures (e.g. 700 0C) in air. These superalloys, such as IN718, are used because of their combination of strength at high temperature and resistance to creep, most notably as components of aircraft engines such as turbine rotor disc parts. SAGBO suggests that crack growth in these superalloys follows the local formation and rupture of brittle oxides known as oxide intrusions, such as NiO and Cr_2O_3, at a grain boundary ahead of the crack. The framework for solving this important engineering problem is described in terms of analytical and computational models that are believed to capture the physical mechanism of the process. In particular, the intrusion is modelled with dislocation loops forming a 2-dimensional triangular object, while the distributed dislocation technique is used to evaluate the stress-field of the system composed of: a mode 1 crack in plane strain, as in the BCS model; the intrusion; and a plastic zone, which is composed of two planar regions inclined to the plane of the crack, beyond the intrusion. The stress state predicted by this model is firstly used to understand the sequence of events in SAGBO and, secondly, to predict the rate of the crack growth. The latter is achieved because the stress-assisted diffusion of oxygen within the intrusion is simulated. Mitigating SAGBO will help to prevent the premature failure of aircraft engines, while also making them more efficient, reliable and less polluting.

(P2.13) **Uncertainty quantification for classical effective potentials**

S Wishart and P Brommer

University of Warwick, UK

Effective potentials are an essential tool in the implementation of classical molecular dynamics (MD) simulations. However, little is understood of the errors incurred in representing the high dimensional configuration space of a material by an effective potential containing considerably fewer parameters. Frederiksen et al. [1] outline the probabilistic, sloppy model method, which enables the implementation of uncertainty quantification (UQ) into the interatomic potential generation process. Uncertainties in the effective potential are propagated through MD to obtain uncertainties in quantities of interest, i.e. cohesive energies, thermal diffusivity or elastic constants. This work aims to implement the sloppy model method in the *potfit* open source force matching code [2] and to build upon the current understanding of UQ through investigation of parameter space sampling efficiency in the *potfit* optimisation algorithms.

[1] S. L. Frederiksen, K. W. Jacobsen, K. S. Brown, and J. P. Sethna. Phys. Rev. Lett., 93(16), 2004

[2] P. Brommer and F. Gahler. Potfit: effective potentials from ab-initio data. Modell. Simul. Mater. Sci. Eng., 15(295-304), 2007

(P2.14) **Modelling chemomechanical materials failure processes in SiC and diamond**

P Patel and J Kermode

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Atomistic simulations of crack propagation are key to understanding the behaviour of materials. Cracks involve strong coupling across the scales, with bond breaking on the quantum scale driven by long range stress fields. Current QM methods have limited simulation sizes in comparison to the sizes required to adequately capture elastic effects. This limitation can be overcome by combining a QM description of the critical part of the system with a classical interatomic model sufficient to reproduce the elastic response [1]. This relies on insensitivity of QM forces to moving atoms far away, i.e. strong force locality. The overall goal is to further coarse grain to the continuum scale while maintaining the overall fracture dynamics.

Applications in covalently bonded single crystals to complex alloys are underway. Screened classical potentials [2] predict a brittle response in both silicon carbide (SiC) and diamond, giving confidence in their applicability. DFT SiC surface energy calculations produced predictions in good agreement with experiment [3]. Neither DFT or MD alone can address complex chemistry such as stress corrosion cracking [4] or impurity effects. Extension of multiscale approach to SiC and diamond, including testing the force locality and simulations of diamond containing nitrogen defects, thought to deflect cracks, are in progress.

[1] N. Bernstein et al., Rep. Prog. Phys. 72, 026501 (2009)
[2] L. Pastewka et al., Phys. Rev. B. 87, 205410 (2013)
[3] G. Sernicola et al., In Prep (2016)
[4] A. Gleizer et al., Phys. Rev. Lett. 112, 115501 (2014)

(P2.15) **A numerical study of non-linear polycrystalline materials through a homogenization technique**

T M Schlittler and R Cottereau

Laboratoire MSSMat – CentraleSupelec, France

In this poster, we will focus on the study of polycrystalline materials, such as most metals and many types of ceramics, using numeric multi-model coupling methods. Different scales and models are associated to these materials, and here we are interested in two of them: a micro scale, where a heterogeneous elasto-plastic model is considered, and a macro scale, with a homogeneous non-linear model.

The motivation of this work is to identify the properties of the macro scale model knowing those of the micro scale model. From the numerical point of view, one can perform a homogenization on the multi-scale system. Such methods are very sensitive to the boundary conditions and to the ratio between the characteristic scales of the models, and can introduce a bias to the resulting homogenized macro scale tensor if this ratio is too high. In the cases where a stochastic model is used to represent the micro scale, this bias is still present even after using an infinite number of Monte-Carlo realizations.

We will present an application of a homogenization which reduces this bias, based on the Arlequin method applied to a polycrystalline material. We will model the micro scale system using a stochastic, non-linear micro scale model and a homogeneous macro scale model, and the results obtained will be compare with those of the literature.

This work benefited from French state funding managed by the National Research Agency under project number ANR-14-CE07-0007 CouESt.

(P2.16) **Multiscale thermo-mechanical modelling of cemented tungsten carbide in hard rock drilling**

D Tkalich[1], G Cailletaud[1], V Yastrebov[1] and A Kane[2]

[1]MINES ParisTech, France, [2]SINTEF Materials and Chemistry, France

The mechanical behavior of drilling tools made of cemented tungsten carbides is investigated in impact interaction with hard rock. Cemented tungsten carbides consist of micro- or nano-sized tungsten carbide (WC) grains embedded in a metal matrix (binder).

Two homogenization methods are considered in the current study. First, a direct two- and three-dimensional finite-element simulations are performed using representative material element (RVE) with an explicitly represented microstructure constructed using modified Voronoi tessellation/Poisson cutting algorithm. Second, a uniform field N-phase model, based on Eshelby's solution of the inclusion problem, was extended to elasto-plasticity by means of a beta-model to represent plastic accommodation. This approach introduces three scales, 1) a macroscopic/structural one, 2) a mesoscopic "composite grain" scale, where the phase is made of one oriented tungsten carbide particle and a certain amount of binder, and 3) the lower scale with carbide and binder. A classical J2 plasticity model is used for the binder phase and a non-associated Drucker-Prager model for the tungsten carbide. Both models use a non-linear isotropic hardening.

Macroscopic finite-element impact simulations with varying incident angles are carried out using the constructed N-phase model in order to obtain stress state evolution at critical locations within the cemented tungsten carbide impactor. Selected stress evolution paths are used as boundary conditions applied to RVE finite-element models, which allows to identify the most dangerous locations within the microstructure, which are responsible for the onset of wear and fracture of the cemented tungsten carbides.

(P2.17) **Diffusion under extreme confinement: finite-size effects in molecular simulation**

P Simonnin[1], B Rotenberg[1], V Marry[1], C Nieto-Draghi[2] and B Noetinger[2]

[1]UPMC, France, [2]IFPEN, France

Fluids transport through nanoporous media is a key issue for unconventional hydrocarbons recovery or for cap rock integrity in the context of CO_2 sequestration. The thermodynamic behavior of a fluid in a clay nanopore depends on the nature of the clay itself and on the physico-chemical effects induced by the confinement. Most studies on the hydrodynamics of confined fluids on the molecular scale are based on model systems such as a Lennard-Jones (LJ) fluid between LJ walls, though some applications to more realistic systems have been published, as water in silica nanopores or between two montmorillonite layers. Such molecular dynamics (MD) simulations are necessary to make the transition from molecular descriptions to continuous ones in order to upscale transport properties from the microscopic to the macroscopic scale.

It is well established that MD calculations of some transport coefficients, such as the diffusion coefficient, can suffer some finite-size artefacts arising from hydrodynamic effects. We recently demonstrated that the shape of the simulation box (anisotropy), that has been ignored so far, also plays an important role. A confined system is by definition anisotropic: In a slit pore, both the physically relevant confining distance and the simulation-required finite lengths in the directions along the surfaces may influence the result. We will discuss the finite-size effects in all directions, for model systems (LJ) and more complex ones (water between clay layers). We will propose an analytical model to determine the effect of finite-size on diffusion coefficient according to the box size.

Symposium D

(D1 invited) **Non-equilibrium first order transition marks the mechanical failure of glasses**

P Schall[1], D Denisov[1], T Dang[1], B Struth[2], A Zaccone[3] and G Wegdam[1]

[1]University of Amsterdam, Netherlands, [2]DESY, Germany, [3]University of Cambridge, UK

Glasses acquire their solid-like properties by cooling from the supercooled liquid via a continuous transition known as the glass transition. Recent research on soft glasses indicates that besides temperature, another route to liquefy glasses is by application of shear that acts as external (mechanical) field, driving relaxation and flow. In this contribution, we show that unlike the continuous glass transition, the failure of glasses to applied stress occurs by a sharp symmetry change that reminds of first-order equilibrium transitions. We use a new combined x-ray and rheology setup to probe the macroscopic theology and the microscopic structure factor simultaneously [1]. Using this setup, we apply oscillatory shear with increasing strain amplitude to probe the yielding of a colloidal glass. When we follow the structure factor as a function of increasing strain amplitude, we observe a sharp symmetry change from anisotropic solid to isotropic liquid structure beyond a critical strain amplitude. Remarkably, this critical strain amplitude corresponds to the crossing point of the storage and loss moduli recorded simultaneously. We observe that concomitantly, intensity fluctuations sharply acquire Gaussian distributions characteristic of liquids. Our observations and theoretical framework identify mechanical failure as a sharp affine-to-nonaffine transition, providing a new conceptual paradigm of the oscillatory yielding of this technologically important class of materials, and offering new perspectives on the glass transition [2].

[1] D. V. Denisov *et al.*, Scientific Reports 3, 1631 (2013)
[2] D. V. Denisov *et al.*, Scientific Reports 5, 14359 (2015)

(D1 oral) **Emergence of cooperativity in plasticity of soft glassy materials**

J Crassous, A Amon, S McNamara and A LeBouil

Université Rennes 1, France

We report an experiment where the emergence of a self-organized plastic flow is observed before the failure. For this we impose an homogeneous stress on a granular material, and measure local deformations for very small strain increments using a light scattering setup. We observe a nonhomogeneous strain that appears as transient bands of mesoscopic size and a well-defined orientation, which is different from the angle of the macroscopic frictional shear band that appears at the failure. The presence and the orientation of those microbands may be understood by considering how localized plastic reorganizations redistribute stresses in a surrounding continuous elastic medium. We characterize the length scale and persistence of the structure. The presence of plastic events and the mesostructure of the plastic flow are compared to numerical simulations.

(D1 oral) **Microscopic origin of the yielding behaviour in metallic glasses in terms of nonaffine stress relaxation and viscous stress build-up**

A Zaccone[1], P Schall[2] and E Terentjev[1]

[1]University of Cambridge, UK, [2]University of Amsterdam, Netherlands

We have proposed an analytical microscopic model based on nonaffine deformations at the atomic level, whereby nonaffine displacements result as a consequence of the local disorder and contribute negatively to the free energy of deformation of the material. The affine contribution, on the other hand, is proportional to the local bonding between atoms (in metals this is controlled by pseudopotentials which also account for many-body effects). The shear induces the breakdown of interatomic bonding in the extension sectors of the solid angle, while new contacts cannot be formed in the compression sectors due to excluded volume, which results in a net decrease of connectivity upon increasing the strain. The theory is successfully tested against experimental data on metallic glasses, and it is able to reproduce the ubiquitous feature of stress-strain overshoot upon varying temperature and shear rate. A clear atomic-level interpretation is provided for the stress overshoot, in terms of the competition between the elastic instability caused by nonaffine deformation of the glassy cage and the stress buildup due to viscous dissipation. Recent modifications of the theory allow us to also describe strain-softening under oscillatory shear and the storage modulus of colloidal glasses glassy polymers as a function of the strain amplitude, which testifies of the universality of the microscopic yielding mechanism upon duly rescaling the relevant size and energy parameters.

(D1 oral) **Thermal fluctuations and elastic relaxation in the compressed exponential dynamics of colloidal gels**

M Bouzid, J Colombo and E Del Gado

Georgetown University, USA

Colloidal gels belong to the class of amorphous systems, they are disordered elastic solids that can form at very low volume fraction, via aggregation into a rich variety of networks. They exhibit a slow relaxation process in the aging regime similar to the glassy dynamics. A wide range of experiments on colloidal gels show unusual compressed exponential of the relaxation dynamical properties. We use molecular dynamics simulation to investigate how the dynamic change with the age of the system. Due to the breaking and the reorganization of the network structure, the system displays stretched or compressed exponential relaxation. We show that the transition between these two regimes is associated with the interplay between the thermal fluctuations and the elastic relaxation. The ballistic behaviour rises from the non local relaxation of internal stresses mediated by a series of “micro-collapses”, on the other hand when the thermal effects dominate, they involve short range displacement and lead to a stretched relaxation.

(D2 invited) **Mesoscopic modeling - specific ingredients and emergent behaviours**

K Martens

Université Grenoble Alpes & CNRS, France

In this talk I will discuss several mesoscopic approaches, such as lattice models and mean-field descriptions for the yielding transition and the non-linear rheology of driven yield-stress materials. Despite the fact that this type of models require some phenomenological ingredients, notably the detailed local yielding rules, they have been shown to match several aspects of the mechanical response very well, such as avalanche statistics, mechanical noise descriptions and rheological features. Further the mesoscopic approach provides an ideal tool to test basic assumptions for different flow phenomena and can serve as a bridge to large scale descriptions of the complex yielding dynamics.

(D2 oral) **Elasto-plastic automata with realistic near field interactions: avalanches and diffusion**

B Tyukodi[1], C Maloney[2] and D Vandembroucq[1]

[1]ESPCI ParisTech, France, [2]Northeastern University, USA

We present results on an elasto-plastic automaton model of an athermal amorphous solid under shear. We study four different variants of the model with two different loading geometries and two different stochastic prescriptions (random yield thresholds or random strain amplitudes). We perform a finite size scaling analysis for the avalanche size distribution and single-site displacement and strain statistics. The avalanche size distribution in all four cases is inconsistent with mean-field depinning results. For three of the four variants, the distribution is consistent with previous results from atomistic simulations and other related elasto-plastic models. The fourth seems to exhibit different scaling properties and may lie in a different universality class. The mean-squared displacement exhibits a pronounced dependence on the microscopic ingredients of the model and is completely non-universal. These results show that while certain microscopic ingredients of the model may be irrelevant for the individual avalanches, they may exhibit a profound impact on long-time correlations and long-lived shear localization.

(D2 oral) **Avalanche phenomena and shear localization near the fracture limit of amorphous solids**

D Fernandez-Castellanos, S Sandfeld and M Zaiser

Institute of Materials Simulation (WW8), FAU, Germany

The plastic behaviour of bulk metallic glasses (BMGs) at room temperature is characterized by strong shear localization after yield, leading to quasi-brittle fracture. However, there is evidence of high plastic deformation at the microscopic scale in form of intermittent flow, known as avalanches. A key challenge in understanding the plastic behaviour of BMGs is to establish statistical links between the microscopic avalanches and the macroscopic brittleness.

To this end, it is useful to coarse-grain the important aspects from the atomistic scale in a mesoscopic model without fully resolving the atomic motions, being thus computationally more efficient. A common approach is to consider plastic activity as a sequence of spatially and temporally localized events, known as shear transformations. Amorphous plasticity arises as a stochastic phenomenon, consequence of the elastic interaction of a large number of shear transformations, whose self-organization together with strain softening leads to the formation of macroscopic shear bands that results in specimen failure.

Using a finite element-based elastoplastic model which for the first time accounts for multi-axial stress states and pressure dependence in a stochastic model of shear transformation activation, we simulate the processes that lead to failure in finite size samples. We characterize the failure process with statistical measures and find that, under creep conditions, the avalanches become power-law distributed with near-mean field behavior as the fracture strain is approached, even at stresses well below the zero-temperature flow stress. We study how loading conditions, temperature and strain softening affect the avalanche statistics and the shear localization process.

(D2 oral) **Reducing the gap between real particle rearrangements and idealized shear transformations in deformation models for amorphous solids**

A Nicolas[1], F Puosi[2], J Rottler[3] and J-L Barrat[2]

[1]CNRS & Univ. Paris-Sud, France, [2]Université Grenoble-Alpes, France, [3]University of British Columbia, Canada

The deformation of amorphous solids involves rapid localised rearrangements of particles, known as shear transformations, which burst out in an elastic medium. These rearrangements are the main building blocks of virtually all mesoscale rheological models. However, they are usually described in a highly idealised way.

We start by characterising the rearrangements observed in molecular dynamics (MD) simulations of a binary Lennard-Jones glass and find considerable deviations from the idealised picture: rearrangements differ widely in size and shape, their shear directions (i.e., the angles of yield) are broadly distributed around the macroscopic shear direction, and the local transformations are not pure shear.

We then turn to the effect of these transformations on the surrounding (elastic) medium. Usually, in mesocopic models, the elastic deformation that they induce is computed under very coarse assumptions, including the uniformity of the medium and the neglect of all inertial effects. We improve on this description by proposing a very simple Finite-Element-based method, which captures the effects of elastic heterogeneity as well as inertia. In particular, we show how the material parameters used as input in the model (namely, the elastic constants and the microscopic viscosity) can be directly extracted from an atomistic MD system. The elastic response to an imposed shear transformation is then computed and good agreement is found between the Finite-Element simulations and the MD results, in terms of disorder-averaged response and fluctuations [1].

[1] Nicolas, A., Puosi, F., Mizuno, H., & Barrat, J.-L. *Journal of the Mechanics and Physics of Solids* (2015)

(D2 oral) **Creep and onset of flow in amorphous solids**

S Merabia and F Detcheverry

CNRS and University Lyon 1, France

Creep is observed in a variety of amorphous solids including among others polymer glasses, metallic glasses and gels. Typically, the strain first increases with time following a power law regime often called Andrade creep. This regime is interrupted by fluidization, after an elapsed time which increases with the applied stress.

Here, we characterize creep and fluidization on the basis of a mesoscopic viscoplastic model, where the mechanical response of the system is characterized by a broad distribution of energy barriers, which may be lowered under the effect of a local deformation.

We show that Andrade creep is accompanied by local strain-hardening driven by stress redistribution. We discuss the effect of aging on the fluidization regime, and the appearance of transient shear bands.Finally, we characterize the effective energy barriers distribution in the steady state regime, after the onset of flow.

(D3 invited) **Stress state effects on non-affine displacements and strain hardening of a metallic glass**

T Hufnagel

Johns Hopkins University, USA

Recent investigations into the mechanical behaviour of metallic glasses have revealed two unusual effects. In the first, an apparent length-scale dependence of elastic strain has been interpreted as evidence of non-affine atomic displacements during nominally elastic loading. In the second, strain hardening has been reported during notched tensile tests, with the hypothesis that a hydrostatic state of tensile stress induced in these specimens promotes annihilation of excess free volume by a diffusional relaxation mechanism.

In this talk we will present results of recent high-energy x-ray scattering, absorption, and imaging studies performed in situ during tensile testing of notched specimens. From the scattering data we are able to determine the effect of the hydrostatic component of stress on the length-scale dependence of strain and thus on the non-affine atomic displacements. From the imaging and absorption measurements we are able to map out the density of the glass under load in order to discern the effect of the hydrostatic component of stress on diffusive annihilation of free volume. The significance of these results for our understanding of atomic-scale mechanisms of deformation of metallic glasses, and of disordered materials more generally, will be discussed.

(D3 oral) **Metadynamics of slow deformation and flow: Time-dependent amorphous plasticity (creep)**

S Yip, P Cao, A Kushima and M Short

Massachusetts Institute of Technology, USA

Rate-dependent phenomena in mechanical behavior are particularly vexing challenges to multiscale simulation because they are beyond the reaches of traditional molecular dynamics. We study tensile strain evolution in a model metallic glass by metadynamics simulation at experimental time scales [1]. Transition-state pathways across an energy landscape with multiple minima and saddle points are sampled to observe three stages of creep behavior, transient (logarithmic in time), steady-state (linear), and tertiary (diverging). The corresponding atomic configurations at each stage reveal the presence of two types of elementary processes in sustaining deformation and flow, independent nucleation of local shear transformations and concerted formation and growth of nanoscale shear bands. Experimentally observed temperature and stress effects on the strain rate are thus explained through molecular calculations using a generic interatomic potential with no empirical assumption or experimental input. Significance of our findings to other phenomena of slow dynamics, notably cement setting [2], stress corrosion cracking [2], and irradiation void swelling [3], will be discussed.

[1] P. Cao, M. Li, R. J. Heugle, H. S. Park, and X. Lin, Phys. Rev. E86, 016710 (2012)
[2] S. Yip and M. P. Short, Nature Materials 12, 774 (2013)
[3] M. P. Short and S. Yip, Current Opinion in Solid State and Materials Science 19, 245 (2015)

(D3 oral) **Shear bands and energy dissipation in metallic and network-forming glasses**

R Jana and L Pastewka

Karlsruhe Institute of Technology, Germany

Molecular Dynamics simulations (MD) were used to study nucleation and propagation of shear bands during simple shear deformation and indentation of CuZr binary bulk metallic glasses (BMG), amorphous silicon (a-Si) and amorphous carbon (a-C). We find that the initial shear bands in a-Si and a-C are more localized than those found in CuZr. This localization is also found in the spatial displacement-displacement correlation function before the onset of shear-banding. We find that thermal effects influence the shear localization, as shear bands vanish at elevated temperatures even below the glass transition temperature. Subsequently, energy dissipation mechanisms in simple shear and indentation were analysed with respect to energy stored in structural changes and energy lost in phononic thermalization. We show a correlation of shear band evolution and dissipated energy fractions over. This connection also holds true at higher temperatures until the shear bands vanish.

(D3 oral) **Yield cirteria developed using atomic scale simulations**

G Molnar[1], Etienne Barthel[2], Anne Tanguy[3], Patrick Ganster[1], Guillaume Kermouche[1]

[1]Ecole des Mines de Saint Etienne, France, [2]ESPCI ParisTech, France, [3]LaMCoS INSA, France

The study deals with the analysis of the plastic response of sodium silicate glasses. We propose a new method using atomistic simulations combined with coarse-grained analysis to calculate structural and mechanical properties at different scales.

The numerical simulations were performed on large samples, and the results were compared to experiments (neutron scattering, NMR, Brillouin scattering).

The systems were tested by deforming the periodic simulation box in a homogeneous way. During compression or tension the dimensions of the simulation box was reduced by a constant displacement step while the positions of the particles were rescaled in a homogeneous way. After the box displacement a new equilibrium position was searched using the Polak-Ribiere conjugate gradient algorithm.

Combining quasi static shear and compressive mechanical deformation, we were able to reconstruct hardening yield surfaces in the 3D stress space, parameterized by the residual shear strain and densification.

After identifying the smallest scale where the material could be considered homogeneous and isotropic we were able to develop continuum based material models.

The observed mechanical response was described using a pressure dependent, hydrostatic hardening yield surface. The functions were then implemented in a finite element code. This way the microscopic results could be compared with mesoscopic real life experiments such as nanoindentation.

(D4 invited) **Universality of avalanche exponents in amorphous plasiticity**

Z Budrikis[1], D F Castellanos[2], S Sandfeld[2], M Zaiser[2] and S Zapperi[3]

[1]ISI Foundation, Italy, [2]FAU University of Erlangen-Nuremberg, Germany, [3]University of Milan, Italy

When subject to loading, amorphous materials exhibit a rich variety of collective phenomena, such as strain localization, intermittent dynamics and power-law distributed avalanches. Avalanches in these systems have received considerable attention, both theoretical and experimental, because their statistics can be used to determine the universality class of the transition to flow in the material. However, the nature of the universality class has been controversial, with disagreement among workers on whether the dynamics can be captured by mean field models.

We present a new fully-tensorial coarsegrained model in 2D and 3D, and discuss avalanche statistics and strain patterning. We demonstrate that the exponents describing avalanche distributions are universal under a variety of loading conditions, system dimensionality and size, and boundary conditions. In all cases, our results are inconsistent with mean field theory.

(D4 oral) **Avalanche statistics when approaching (or leaving) the yielding transition of amorphous solids**

C Liu, E Ferrero, F Puosi, J-L Barrat and K Martens

Universite Grenoble Alpes, France

We study the stress time series caused by plastic avalanches in athermally sheared disordered materials above the yielding transition. Using a mesoscopic elastoplastic model in two and three dimensions, we analyse system size and shear-rate dependence of the stress-drop duration and size distributions, together with their average temporal shape. Close to the transition, we find critical exponents different from mean-field predictions, and a clear asymmetry for individual avalanches. We probe scaling relations for the rate dependency of the dynamics and we report a crossover towards mean-field results for strong driving. We link this crossover with a progressive vanishing of correlations --manifested in the gaussianization of hitherto non-trivial stress fluctuations-- as we increase the drive and depart from the yielding point, alike equilibrium critical phenomena.

(D4 oral) **Role of inertia in the rheology of amorphous systems: a finite element based elasto plastic model**

K Karimi and J-L Barrat

University of Grenoble, France

A simple Finite Element (FE) analysis with varying damping strength is used to model the athermal shear rheology of densely packed glassy systems at a continuum level. We focus on the influence of dissipation on bulk rheological properties. Our numerical studies, done over a wide range of damping coefficients, identify two well-separated rheological regimes along with a cross- over region controlled by a critical damping. In the overdamped limit, inertial effects are negligible and the rheological response is well described by the commonly observed Herschel-Bulkley equation. In stark contrast, inertial vibrations in the underdamped regime prompt a significant drop in the mean-stress level, leading to a non-monotonic constitutive relation. The observed negative slope in the flow curve, which is a signature of mechanical instability and thus permanent shear-banding, arises from the sole influence of inertia.

(D4 oral) **Universality of slip avalanches in flowing granular matter**

D Denisov[1], K Lorincz[1], J Uhl, K Dahmen[2] and P Schall[1]

[1]University of Amsterdam, Netherlands, [2]University of Illinois at Urbana Champaign, USA

The search for scale-bridging relations in the deformation of amorphous materials presents a current challenge with tremendous applications in material science, engineering and geology. While generic features in the flow and microscopic dynamics support the idea of a universal scaling theory of deformation, direct microscopic evidence remains poor.

We study the evolution of slowly sheared granular systems deforming via discrete strain bursts (slips). The granular sample consisting of 10^5 hard spheres is subjected to applied shear and studied with the combination of two techniques – precise stress-strain measurements and 3D laser sheet imaging. Fluctuations in the stress-strain profile allow us to calculate the magnitude of small internal slip avalanches occurring in the sample due to the shear. 3D laser sheet imaging allows us to visualize each individual slip event, estimate its spatial distribution and connect it to fluctuation in the stress-strain curve. By combining macroscopic force fluctuation measurements with internal strain imaging, we demonstrate the existence of robust scaling relations from particle-scale to macroscopic flow [1]. We identify consistent power-law relations truncated by systematic pressure-dependent cut-off, in agreement with recent mean field theory of slip avalanches in elasto-plastic materials, revealing the existence of a mechanical critical point. These results experimentally establish scale-bridging relations in the flow of matter, paving the way to a new universal theory of deformation.

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(D5 invited) **Making a jammed emulsion flow: local rearrangements and correlated motion**

E Del Gado[1], V Venkatesh[1], S Dutta[2] and D Blair[1]

[1]Georgetown University, USA, [2]University of Maryland, USA

Long range correlations and heterogeneities in local strains tend to emerge in jammed materials that are forced to flow, coupled or not to flow instabilities. I'll discuss how non-equilibrium molecular dynamics simulations of model systems can be used to investigate and rationalize different phenomena observed in experiments. In particular, we have used a numerical study to rationalize recent confocal microscopy and rheology experiments on jammed athermal emulsions under shear, which could access the droplets rearrangements. Once the background flow is subtracted, the mean squared displacement of the droplets at first suggests that the non-affine motion might be diffusive in nature. The simulations insight combined with a more quantitative analysis of local rearrangements at small accumulated strains allows us to identify the elementary non-affine rearrangements which underlie the flow. We find evidence that different type of correlated flow events underlie the unjamming of the emulsion at high and low shear rates. At high rates we recognize the coordinated motion of small clusters of droplets moving along the same direction. At low shear rate the elementary non-affine rearrangements are associated to much larger correlated domains, with a complex spatio-temporal correlation pattern, and bear signature of the long range elasticity of the emulsion. I'll also discuss how self-stress states developed in the jammed emulsion at rest may be crucially related to the onset of transient flow instabilities such as banding.

(D5 oral) **Vibrational properties of amorphous materials, and application to nanocomposites**

A Tanguy[1] and V Giordano[2]

[1]INSA, France, [2]Université Lyon 1, France

Vibrational properties of amorphous materials are still poorly understood, due the large amount of disorder at all scales in these materials. However they give rise to an anomalous low-frequency density of vibrational states, also referred to as the Boson peak and responsible for anomalous low temperature dependence in the heat capacity. Morover, high attenuation of low-frequency wave-packets induces a low heat conductivity. We combined a complete analysis of the vibration modes, dynamical structure factor, and energy diffusivity in different models of amorphous materials, to propose a solid but schematic description of the different vibrational regimes, in connexion with different thermal properties. Moreover, we applied the same analysis on nanocomposite materials made of nanocrystalline spherical inclusions embedded in an amorphous matrix. We have shown evidence of the effect of the rigidity contrast between the inclusions and the matrix, on waves propagation in the different regimes mentioned above.

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[2] Damart, T., Giordano, V. and Tanguy, A. (2015). Nano-crystalline inclusions as a low-pass filter for thermal transport in amorphous silicon. Physical Review B, Vol. 92, p.094201

[3] Beltukov, Y., Fusco, C., Parshin, D.A. and Tanguy, A. (2015). Boson peak and Ioffe-Regel criterion in amorphous silicon-like materials: the effect of bond directionality. Condmat: arXiv:1510.01761. Physical Review E (February 2016)

[4] Shcheblanov, N., Mantisi, B., Umari, P. and Tanguy, A. (2015): Detailed Analysis of Plastic Shear in the Raman spectra of SiO_2 glass. Journal of Non-Crystalline Solids, 428, p.6-19

(D5 oral) **Confinement effects on the correlations of plasticity**

F Varnik[1], M R Hassani[1] and D Raabe[2]

[1]Ruhr-Universität Bochum, Germany, [2]Max-Planck-Institut für Eisenforschung, Germany

Solid walls may strongly alter the spatio-temporal correlations of plastic activity. Via large scale MD simulations of a model glass, we show that wall effects are manifest in two distinct ways. On the one hand, walls slow down the dynamics of single particle motion and the rate of plastic rearrangements in their immediate vicinity. On the other hand, this is accompanied by a larger stress release during a plastic rearrangement and stronger in-plane correlations of plastic activity [1], an effect also visible at larger distances from the wall [2]. These findings are rationalized within recently developed mesoscopic elasto-plastic models [3]. Various tests and comparisons with continuum mechanics calculations are also provided which underline the reliability of the underlying simulations and the obtained results.

[1] F. Varnik, S. Mandal, V. Chikkadi, D. Denisov, P. Olsson, D. Vagberg, D. Raabe, and P. Schall, Correlations of plasticity in sheared glasses, Phys. Rev. E 89, 040301 (2014)

[2] M. Hassani, D. Raabe and F. Varnik, Wall effects on the correlations of plasticity (submitted to EPL)

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(D5 oral) **Rheology of weakly attractive systems: the role of energy dissipation**

E Irani[1], P Chaudhuri[2] and C Heussinger[1]

[1]University of Goettingen, Germany, [2]Institute of Mathematical Sciences, India

The rheological response of a particulate system with attractive interactions is studied using different models for the dissipation of energy. In systems with the damping force directed normally to the contact point, attractive interactions result in a finite yield stress, and an iso-static structure emerges below the jamming point with shear bands forming as a consequence of non-monotonic flow curves. On the other hand, tangential damping gives rise to the monotonic flow curves and a viscous flow develops in the overdamped regime. However in that case, decreasing the damping factor introduces the inertial time-scale, leading again to non-monotonic flow curves and inertia-induced shear-banding is observed in the underdamped regime. In both cases, the rheology of the system is expressed in terms of relevant damping time-scales and the ratio of dissipative to elastic forces.

(D5 oral) **From kinetics to rheology in inertial granular flows**

E DeGiuli and M Wyart

Ecole Polytechnique Federale de Lausanne, France

Dense flow of granular materials is strongly constrained by steric effects, which introduce new velocity and strain scales into flow. As the inertial number I tends to zero, kinetic quantities have a singular behaviour: compared to the affine velocity scale, D \dot ε, where D is particle size, steric constraints cause the velocity fluctuations, V, to diverge. At the same time, the characteristic strain scale associated to velocity decorrelation, ε_v, vanishes. We report numerical simulations showing power-law behaviour of V/(D \dot ε) and ε_v, for both frictional and frictionless particles. We show that these observables, together with considerations of energy dissipation, lead to a phase diagram that distinguishes frictional from frictionless flows, and we furthermore show how these scaling's can be derived using geometrical arguments. In the frictionless case, these results are crucial in obtaining the singular behaviour of the rheology, μ(I). Finally, we compare and contrast the situation for frictionless and frictional particles, summarizing the outstanding problems.

(D6 invited) **Microscopic dynamics and macroscopic rheology in a semi-crystalline polymer**

L Cipelletti[1], Y Nagazi[1], G Brambilla[2], G Meunier[2], P Marguerès[3] and J-N Périé[3]

[1]University Montpellier, France, [2]Formulaction, France [4]Institut Clément Ader, France

We couple conventional extensional rheometry and light scattering methods to investigate simultaneously the mechanical properties and the microscopic dynamics of polyether ether ketone (PEEK), a semi-crystalline polymer, and of other polymer-based amorphous materials. Space-resolved diffusing wave spectroscopy, a recently introduced dynamic light scattering method, allows us to generate a spatial map of the sample dynamics on length scales ranging from a fraction of nm to tens of nm. A simple relation is found between the macroscopic stress relaxation at a fixed strain and the temporal evolution of the microscopic dynamics. Moreover, the microscopic dynamics is found to speed up dramatically as the material is increasingly strained. Remarkably, such acceleration occurs well before any macroscopic or mesoscopic indication that the material is close to its rupture limit.

(D6 oral) **Influence of deformation induced topological anisotropy on mechanical properties of silica glass: An atomistic study**

E Bitzek[1], S Ganisetti[1] and J Horbach[2]

[1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany, [2]Heine-Universität Düsseldorf, Germany

Glasses are generally believed to be isotropic materials. However, it is well known that anisotropy can be introduced in silica glass, e.g., by wire drawing, and that the mechanical properties are subsequently anisotropic. Since topology plays an important role for the mechanical properties, it is necessary to understand the physics behind the development of topological anisotropy on the atomic scale. Here we present the results of atomistic simulations using an ab-initio based polarisable force field. Isotropic silica glass was prepared by the melt quenching method. Anisotropy was introduced at different temperatures by either elongating, compressing or shearing the glass at different rates. During load, transient anisotropy is observed, as characterized by the anisotropy factor. Significant persistent anisotropy, which remains after load removal, could only be introduced by compression and shear. The conditions favourable to the formation of persistent anisotropy, the underlying mechanisms and the relationship between transient and persistent anisotropy are analysed in detail. Samples with persistent topological anisotropy also show a pronounced anisotropy in the mechanical properties, in particular on the elastic constants and fracture strain. The results are compared to simulations on bulk metallic glasses and discussed in the framework of mesoscale and continuum models for the deformation of amorphous materials.

(D6 Oral) **Small-scale mechanical response and dynamical behaviour of a model amorphous silicon solid**

C Fusco[1], T Albaret[2] and A Tanguy[1]

[1]INSA, France, [2]Université Lyon 1, France

We present a study of the atomic-scale response of a model amorphous silicon sample subjected to a shear deformation. The dynamical mechanical behaviour of the system is investigated by Molecular-Dynamics simulations both at finite shear deformation rates and in the limit of a quasi-static shear regime. Our model allows us to vary the degree of local order of the amorphous system by playing on a specific parameter of the interatomic interactions in order to understand the effect of the atomic-scale structure on the mechanical response.

The mechanical behaviour of the system is rather heterogeneous even in the elastic regime where we observe the nucleation of irreversible atomic rearrangements. These rearrangements grow with the applied deformation and result in large plastic events or shear bands throughout the sample. Noticeably, in the quasi-static regime the spatial correlation between local plastic rearrangements and structural defects increases as a function of the local order.

At finite shear rates the flow stress in the plastic regime follows a power-law behaviour as a function of the strain with an exponent close to 0.5 only slightly dependent on the local order. Interestingly, the apparent viscosity can be related to a single relevant time scale characterizing the collective motion of large clusters of atoms (-relaxation). This suggests a universal strong connection between the local dynamics and the global mechanical behaviour, rather independent of the fine details of the local structure, which can be explained by the nucleation and the avalanche-like propagation of atomic rearrangements.

(D6 oral) **Mapping between atomistic simulations and Eshelby inclusions in the shear deformation of amorphous Silicon**

F Boioli, T Albaret and D Rodney

University of Lyon1, France

Low ductility in amorphous solids is a consequence of the localization of the plastic deformation in shear bands, which leads to catastrophic failure. As a consequence, understanding the localization of plastic deformation and the formation of shear bands is of utmost importance. Generally, it has been accepted that local irreversible rearrangements of small clusters of atoms, Shear Transformations (STs), are the elementary processes involved in the deformation of amorphous systems and several mesoscale models based on STs have been proposed. Still the fundamental mechanisms underlying ST occurrence and shear bands formation are not yet clear. In this context, atomistic simulations can provide significant details that would otherwise be unavailable.

In this work we investigate amorphous silicon by performing quasi-static shear simulations with Stillinger-Weber type potentials. First, the analysis of the shear simulations allow to identify local plastic rearrangements. By fitting their displacement field on collections of Eshelby spherical inclusions, we characterize their size and plastic strain and show that these two ingredients with a measure of the strain-dependent shear modulus suffice to reproduce the atomistic stress-strain curve with fidelity. This result justifies the usual decomposition of plastic rearrangements into STs as used in mesoscale simulations and provides atomic-scale parameters to characterize the local shear rearrangements needed to build such models. Second, using the Nudged Elastic Band method, we calculate the energy barriers and the activation volumes involved in the plastic rearrangements, thus accessing the strain-rate sensitivity of the glass plasticity, another important parameter for mesoscale models.

(D7 invited) **Avalanche phenomena in a sheared granular layer coupled to soft elastic plates**

R Ecke, D Geller and S Backhaus

Los Alamos National Laboratory, USA

We present stick-slip statistics and real-time dynamics from a granular layer enclosed between two soft compliant boundaries in which one of the boundaries is fixed while the other is translated at very low strain rate. The qualitative spatial distribution of normal and tangential forces acting upon the boundary is indicated by an optical birefringence technique, quantitative local strain measurements are obtained from elastic displacements at the boundary, and global forces are used to investigate short-time dynamics. These probes yield an excellent characterization of the heterogeneous distribution of motion involved in the stick-slip behaviour of the granular layer. In particular, we observe power-law scaling, with exponent -3/2, of the distribution of small displacement moments whereas large, system-size events are Log-normally distributed [1]. The motions of the granular constituents are also obtained and are strongly correlated with boundary motion. We consider both the fast and slow dynamics of the system from the perspective of an effective friction coefficient and from the point of view that the slip events represent a brittle fracture of the granular layer. We make close comparison with statistical physics models of avalanche behavior and relate our results to naturally occurring earthquake phenomena.

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(D7 oral) **Yielding and flow properties of vibrated granular media**

O Dauchot[1], M Van Hecke[2], G Wortel[3] and R Candelier[4]

[1]UMR Gulliver, CNRS, ESPCI Paris, France [2]AMOLF, Netherlands, [3]Leiden University, Netherlands, [4]CNRS, France

In the recent years many aspects of the rheology of athermal, macroscopic grains and that of Brownian colloidal suspensions have been clarified. Several issues remain however actively debated regarding the crossover between the athermal and thermal regimes as well as the role of friction.

In this talk I will present several experimental results regarding the yielding and the flow properties of *shaken* grains, the vibration being a way to mimic the effect of temperature, while avoiding possible complications related to hydrodynamics interactions. On one hand I will review the observations made when probing the mechanics and local rheology of a vibrated monolayer of disks close to the jamming transition. Here the dominant features are the presence of very large spatial correlations, strongly intermittent dynamics and critical avalanches. On the other hand I will show that the macroscopic rheology of a gently shaken granular layer also exhibits critical fluctuations, albeit of a complete different kind : they are maximal at some finite flow rate and finite vibration amplitude, away from the yielding transition. These observations can be understood in terms of a self-induced activation, which add to the externally provided vibration. Finally I would like to discuss whether our understanding of Brownian colloidal suspension allows to better understand the intriguing features reported in the case of vibrated grains.

(D7 oral) **Mechanical instabilities in granular media induced by non-linear acoustic waves.**

J Leopoldes, A Tourin and X Jia

ESPCI, France

Soft glassy solids liquefy above a shear threshold called the yield stress. In the case of granular materials, this corresponds to a mechanical instabilitiy involved in avalanches and earthquakes. Here, we study the effects of impinging acoustic waves on such instabilities at the laboratory scale. Above a critical amplitude, the sound-matter interaction becomes irreversible and the wave velocity, correspondingly the elastic modulus, decrease. This is due to the strong modification of the force network without any rearrangement of the grains, as shown by the correlation function of the multiply scattered Coda waves [1]. We then show that far below the static threshold, the onset of sliding at solid contacts is triggered by nonlinear sound waves, due to the acoustic lubrication of the contact area between grains, which reduces the apparent coefficient of friction [2]. We illustrate the consequences of such a mechanism by a series of experiments where a granular layer brought to an inclination below to the angle of repose is destabilized by acoustic waves [3]. Such an avalanche triggered by small vibration amplitudes proceeds because of the decreased friction between the particles, while dilatancy [4] is not affected.

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(D7 oral) **Suppression of the threshold of a granular solid by mechanical fluctuations**

A Amon[1], A Pons[2], T Darnige[2], J Crassous[1] and E Clément[2]

[1]Université Rennes 1, France, [2]PMMH, France

For a granular material, when the ratio between the shear stress and the confining pressure is smaller than the Mohr-Coulomb threshold, the system can be considered as a solid. Nevertheless, a long-term creep is observed in this solid phase in stress imposed experiments. This creep process is the result of the accumulation of localized plastic events and can be interpreted using a generic model taking into account aging of the system and rejuvenation due to the shear rate.

We present recent experimental and theoretical results demonstrating that, even very far from the threshold, the superposition of tiny modulations to the imposed stress are sufficient to change the response of the system from a logarithmic creep to a linear one. Thus, observed on a long enough time, the granular solid behaves in fact as a liquid. We give a theoretical interpretation of this fluidization without invoking an effective temperature due to a mechanical noise. We interpret our observations as a secular effect, i.e. a ratcheting process which is revealed only on very long time. We study experimentally the spatial repartition of the plastic processes at the origin of the observed creep and show that a local fluidity model is sufficient to interpret fully all our experimental observations.

(D7 oral) **Shear cessation in Brownian-dynamics simulation for 2D hard disks**

S Fritschi[1], T Voigtmann[2] and M Fuchs[1]

[1]University of Konstanz, Germany, [2]Heinrich Heine University Düsseldorf, Germany

Residual stresses strongly affect the mechanical properties of glass and thus are widely used, but remain poorly understood. We study the fundamental structural process causing homogeneous residual stresses in glass-forming colloidal dispersions [1]. Brownian-dynamics computer simulations capture the nonequilibrium transient dynamics after the cessation of shear flow [2]. In glassy states persistent residual stresses are found that depend on the flow history. The partial decay of stresses from the steady state to this residual stress as well as the decay of density correlations onto a finite long time plateau are governed by the previous shear rate. Using a glassy hard-disk system, we also link this macroscale dynamics to microscopic particle motion, monitoring the transient displacements, radial distribution functions, local strains and stresses measured during the relaxation from the steady state. A flow-induced second plateau is found in the mean-squared displacement at long times. For sufficiently small previous shear rates we observe a rich structural relaxation after the interruption of the flow. Phenomena like collective, avalanche like displacements associated with a sudden stress relaxation and high local stresses and strains are observed.

[1] M. Ballauff, J. M. Brader, S. U. Egelhaaf, M. Fuchs, J. Horbach, N. Koumakis, M. Krüger, M. Laurati, K. J. Mutch, G. Petekidis, M. Siebenbürger, Th. Voigtmann, and J. Zausch, Phys. Rev. Lett. 110, 215701

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(D8 invited) **Cooperative phenomena in the mechanical behaviour of filamentous materials with molecular motors**

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Biological cells sense and respond to mechanical stimuli in a rather intricate manner. Indeed, cell mechanosensing involves the interplay of several cytoskeletal constituents, primarily filaments, such as actin microfilaments or microtubules, crosslinking proteins, and molecular motors. Moreover, mechanical forces are known to be shared between molecular motors such as myosins and different actin crosslinkers. Here we report cooperative behaviour as a result of motor reorganizations under mechanical cell deformation. In our study we mainly use the worm-like chain as the starting model to characterize the cytoskeletal filaments and we apply different Monte Carlo techniques, from the Metropolis algorithm to biased sampling, to statistically characterize the mechanical response of several filaments under various modes of deformation. Different types of cell deformation trigger distinct responses, with molecular motors responding or reacting against length dilation or shear. The reversible nature of crosslink binding in conjunction with motor dynamics and the non-affine deformation of the filaments leads, for instance, to collective phenomena such as sudden and discontinuous unbinding processes, characteristic of a first order transition. Our observations help to determine the influence of motor behaviour on the collective system response.

(D8 oral) **Delocalized plastic flow in proton-irradiated monolithic metallic glasses**

S Ryu, J Heo, S Kim and D Jang

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Creating new materials with novel properties through structural modification is the Holy Grail of materials science. The range of targetable structures for amplification of mechanical properties in metallic glasses would include types of atomic short range orders at the smallest scale through compositions or morphologies of phases in composites. Even though the usefulness of the latter approach has been successfully demonstrated in the past decades1,2, the feasibility of the former has been incompletely proved with only marginal property improvements reported within experimentally-accessible atomic-level structural changes. Here, we report the significant enhancement of deformability in Zr-based monolithic metallic glass only through the atomic disordering by proton irradiation without altering any other structural traits. Metallic glass nanopillars that originally failed catastrophically without any notable plasticity become capable of attaining more than 30% uniaxial plastic strain accommodated by homogeneous deformation when irradiated to 1 displacement per atom (DPA). By combining molecular dynamics simulations and nanoindentation experiments, we discuss the atomistic origin of this improved plasticity in terms of density and spatial distributions of icosahedral short range order influenced by irradiation. The enhanced plasticity is explained in light of the changes in the icosahedral network topology and vibrational modes that are induced by proton irradiation.

(D8 oral) **Combining continuum mechanics with microscopic descriptions of nonlinear glassy rheology: Hybrid-Lattice Boltzmann simulations**

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German Aerospace Center, Germany

The dynamics of soft glassy matter close to the glass transition is characterized by a wide range of timescales and resulting memory effects. The interplay of this dynamics with spatially smooth flow fields gives rise to nonlinear rheological phenomena. A microscopic description is provided by the mode-coupling theory of the glass transition, in the integration-through transients framework (ITT-MCT).

To understand flow, creep and yielding of amorphous materials close to the glass transition, we combine the macroscopic Navier-Stokes equations with constitutive equations provided by the microscopic ITT-MCT. In order to capture the pronounced memory effects in the dynamics, these constitutive equations are nonlinear integral equations spanning many decades in time. We have developed a hybrid-Lattice Boltzmann algorithm [1] that is capable of dealing with this and similar material laws in the regime of high Weissenberg numbers. In the present contribution, results will be discussed for the creep and yielding behaviour in pressure-driven flow of glassy suspensions, and for the formation of residual stresses after the cessation of flow.

[1] S. Papenkort and Th. Voigtmann, J. Chem. Phys. 143, 044512 (2015); J. Chem. Phys. 143, 204502 (2015)

(D8 oral) **Fragility in shear-jammed suspensions**

R Mari and M Cates

University of Cambridge, UK

Dense suspensions can jam under shear when the volume fraction of solid material is large enough. In this work we investigate the mechanical properties of shear jammed suspensions with numerical simulations. In particular, we address the issue of the fragility of these systems, i.e., the type of mechanical response (elastic or plastic) they show when subject to a mechanical load differing from the one applied during their preparation history.

(P1.19) **Strain drop measurements of porous materials probing earthquake dynamics**

V Soprunyuk[1], S Puchberger[1], W Schranz[1], A Troester[2], E Vives[3] and E Salje[4]

[1]University of Vienna, Austria [2]Vienna University of Technology, Austria, [3]University of Barcelona, Spain, [4]University of Cambridge, UK

SiO_2-based porous materials Vycor and Gelsil have been measured under slow uniaxial compression at constant force rates of 0.0001 - 0.001 N/s using a Diamond DMA (Dynamical Mechanical Analyzer, Perkin Elmer). The jerky evolution of the sample's height with time was analyzed in order to determine the corresponding power-law exponents for the maximum velocity distribution, the modified Omori's law as well as the waiting time distribution of events. A comparison with recent results from acoustic emission (AE) data on the same materials [1] shows similitude in the statistics, although the two methods operate on different spatial and temporal scales. Moreover, the obtained power-law exponents are in good agreement with mean-field values. The results demonstrate that the failure dynamics of materials can be well studied by measuring strain drops under slow compression, which opens the possibility to study earthquake dynamics in the laboratory also at non-ambient conditions, i.e. at high temperatures or under confining liquid pore pressure.

The present work was supported by the Austrian Science Fund (FWF) projects P28672-N36 and P27738-N28.

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(P1.20) **Cooperative strings and glassy interfaces**

M Arutkin[1], E Raphael[1], J Forrest[2] and T Salez[1]

[1]ESPCI ParisTech, France, [2]University of Waterloo, Canada

We present a minimal theory of glass formation based on the ideas of molecular crowding and string-like cooperative rearrangements [1]. In the bulk case, we obtain a scaling expression for the number of particles taking part in cooperative strings as a function of density, and we recover the Adam-Gibbs description of glassy dynamics. Then, by including thermal dilatation, the Vogel-Fulcher-Tammann relation is derived. Moreover, the random and string-like characters of the cooperative rearrangements permit the prediction of a temperature-dependent expression for the cooperative length of bulk relaxation. This theoretical picture enables the exploration of the influence of sample boundaries, in various geometries where the system size is comparable to the bulk cooperative length, such as thin supported films[1] and nanoparticles[2] made of polymers. We also discuss important matters such as the glass transition of binary mixtures[3], and the properties of glassy-rubbery polymer interfaces[4].

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[3] Fox Jr, Thomas G., and Paul J. Flory. "Second-order transition temperatures and related properties of polystyrene. I. Influence of molecular weight." Journal of Applied Physics 21.6 (1950): 581-591
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(P1.21) A string model for the boson peak in amorphous materials

F Lund

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It is proposed to apply continuum mechanics to both crystalline materials and their amorphous counterparts, at similar length scales. To this end, the normal modes of a continuum solid endowed with a random distribution of line defects that behave like elastic strings are described. These strings interact with elastic waves in the bulk, generating wave dispersion and attenuation. Explicit formulae are provided that relate these properties to the density of string states. For a density of states that mimicks the Boson peak (BP) in amorphous materials, the attenuation as a function of frequency w behaves as w^4 for low frequencies, and, as frequency increases, crosses over to w^2 near the BP, in agreement with a number of experimental results. A Ioffe-Regel criterion can be satisfied at the BP. Dispersion is negative in the frequency range where attenuation is quartic and quadratic in frequency, with effective velocity reaching a minimum near the BP.

The possibility of linking this model to the microstructure of amorphous materials is discussed. Consistency with the string-like behaviour observed in numerical simulations of soft spheres below the glass transition temperature [1], and of Lennard-Jones [2] and Cu-Zr liquids [3] is observed, provided that, while the atoms move along a string, the string itself moves transversely.

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(P1.23) Random matrix model of amorphous solids

Y Beltukov[1] and D Parshin[2]

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In this work we present a stable random matrix model to describe general vibrational properties of amorphous solids. We take the dynamical matrix in the form $M = A\,A^T + \mu\,M0$ where A is a random matrix and $M0$ is an ordered crystalline part. Since matrix $A\,A^T$ is always positive definite, such form of the dynamical matrix guarantees the mechanical stability of the system for any random matrix A and any positive value of the parameter μ.

We consider a simple cubic lattice with a strong force-constant disorder. Non-diagonal matrix elements A_{ij} between the nearest neighbor atoms are taken as independent Gaussian random numbers with zero mean $\langle A_{ij}\rangle = 0$ and a constant variance $\langle A_{ij}^2\rangle = \Omega^2$. The diagonal elements are calculated as a minus sum of non-diagonal elements $A_{ii} = -\sum_{j\neq i} A_{ji}$. Matrix $M0$ is a crystal dynamical matrix for the same lattice with nonzero matrix elements between the nearest neighbors $M0_{ij} = \Omega^2$.

We show that we can vary the strength of disorder in this model going from extremely disordered soft medium without macroscopic rigidity ($\mu = 0$) to a perfect crystal ($\mu >> 1$). We find the scaling relations of the boson peak frequency, the Ioffe-Regel criterion, elastic moduli, and the lengthscale of non-affine mechanical response. We show that they map directly onto the scaling observed in systems near jamming transition point.

(P1.24) **Linear viscoelastic characterization of heterogeneous, amorphous polymer blends in the megahertz frequency regime with acoustic wave devices**

K Shull[1], L Sturdy[1], D Delgado[1] and C Burkhart[2]

[1]Northwestern University, USA, [2]Goodyear Global Materials Science, USA

This presentation focuses on the development and use of two acoustic techniques that are able to quantify the linear viscoelastic properties of polymeric materials at high frequencies. The first of these is based on use of a bulk acoustic wave device, analogous to the well-known quartz crystal microbalance (QCM), but utilizing films that are sufficiently thick so that their viscoelastic properties at 15 MHz can be quantified. The second technique utilizes a surface acoustic wave device based on a Love wave sensor operating at 120 MHz. This technique does not require the use of thin films and can be used characterize the surface regions of bulk materials, but gives results that are more difficult to quantify. Both techniques enable direct measurement of material properties at a high frequency regime that is typically obtained by time-temperature shifting of data obtained at lower temperatures and lower frequencies. In this presentation we compare shifted values obtained by traditional methods at lower frequencies to direct high-frequency measurements in amorphous polymers, including immiscible blend systems for which time-temperature shifting becomes problematic.

(P1.25) **Atomic-scale study of high-frequency energy dissipation in oxide glasses**

T Damart[1], D Rodney[1] and A Tanguy[2]

[1]ILM, France, [2]LAMCOS, France

The attenuation of high-frequency sound waves in glasses is still poorly understood, partly because the underlying mechanism strongly depends on the frequency of the incident wave and the ratio between its wavelength and the characteristic length scales in the glasses. A better understanding would however highly benefit a number of applications. One example is the coatings of the mirrors used in the interferometers of gravitational wave detectors. The coatings, made of a multilayer of oxide glasses (SiO2 and Ta2O5), are the main sources of dissipation that limit the precision of measurement of the entire detectors.

Here, we investigate energy dissipation in model oxide glasses using atomic-scale simulations. We first study the structural and vibrational properties of SiO2 and Ta2O5 glasses. We then employ Molecular Dynamics to measure energy dissipation using simulated mechanical spectroscopy in the GHz and THz regimes. We find that the numerical models compare favourably with existing experimental data. We also show that when the frequency of the loading lies within the frequency range of the normal modes of the system, dissipation is mainly harmonic and arises from the coupling between the loading and the collective excitations of the system, rather than individual atomic motions. At lower frequencies, anharmonicity is measured and analysed.

(P1.26) Bond breaking in silica glass by water dimer: hybrid quantum-classical simulation

T Kouno, S Ogata, T Tamura and R Kobayashi

Nagoya Institute of Technology, Japan

The silica glass has superior durability and mechanical strength and has expected to be used for the nearly permanent data-storage device. Even in silica glass with relatively high water resistance, substantial amount of Si-OH groups is produced through the Si-O bond breaking reactions by the migrated water. Understanding theoretically both conditions and microscopic mechanisms of the Si-O bond breakings by water is quite essential.
We propose a novel reaction model between the water molecules and silica glass by performing reaction-dynamics simulation using the hybrid quantum-classical simulation method. In the hybrid method, the quantum region treated with the electronic density-functional theory (DFT) is embedded in a large classical system: the quantum and classical regions couple mechanically with each other. We perform the hybrid simulation of a silica glass system (about four thousand atoms) with water molecules inserted in it. We set the quantum region as that composed of the water molecules and their surrounding atoms. For fast computation we use the real-space grid based implemented of the Kohn-Sham DFT (RGDFT) code.

In the cases where a single water molecule exists in the system, we do not observe any reaction between the water and silica atoms even in highly stretched or expanded systems. In the cases where two molecules are placed initially at neighbouring sites, they form a water-dimer in a relatively large site of the silica glass. The water dimer reacts quite sensitively with the silica atoms to break the Si-O bond. Detailed analyses about the reaction mechanisms are presented.

(P1.27) Finite-size effects in a model for plasticity of amorphous composites

T Botond[1], C Lemarchand[2], J Hansen[3] and D Vandembroucq[1]

[1]ESPCI, France, [2]Université Paris-Sud, France, [3]Roskilde University, Denmark

In this talk, the plastic behaviour of a composite material composed of hard or soft inclusions embedded in an amorphous matrix is discussed. In particular, the increase of the flow stress due to hard particles and the change in strain localization due to soft particles are examined. A two-dimensional mesoscopic depinning-like model accounting for Eshelby elastic interactions is used to represent amorphous plasticity. Inclusions differ from the amorphous matrix only by their plastic threshold. First, the reinforcement due to hard inclusions is considered. Numerical results show a complex size-dependence of the effective flow stress of the amorphous composite. The reinforcing mechanisms and their effects on localization are discussed. Plastic strain is shown to gradually concentrate on the weakest band of the system. This correlation of the plastic behaviour with the material structure is used to design a simple analytical model. The latter nicely captures reinforcement size effects in log(N)/N)^(1/2), where N is the linear size of the system, observed numerically [1]. Second, the focus is put on the effect of soft particles inclusion on localization. Depending, on the initial condition, localization can occur in the pure amorphous matrix. Preliminary results show that including soft particles modifies this localization behaviour.

[1] B. Tukyodi, C. A. Lemarchand, J. S. Hansen, D. Vandembroucq, *Finite-size effects in a model for plasticity of amorphous composites*, to appear in Phys. Rev. E.

(P1.28) **Kaiser effect in porous materials**

A Guarino

Université de la Réunion, France

We present here a dynamicspring-network model to study the Kaiser effect of a porous media submitted to a time-dependent stress. In the model, the porosity is represented by missing springs. Thermal fluctuations introduce dynamics in the model.

The Kaiser effect, which is the fact that that the acoustic emissions of a stressed sample is zero if the applied stress is smaller than a previously applied one, is well known since the '50s. This effect has been observed in metals, rocks, and for heterogeneous materials as wood and fiberglass. In order to check the behavior of our model with respect to the Kaiser effect, we have imposed periodic forces to the spring network. We found that if KT=0, no microckaks are observed after the first period. Conversely, if KT > 0, spring failures are produced after the first on every cycle. We compared our numerical results with experimental datas from fiberglass and wood fracture experiments.

(P1.29) **A computational framework for discrete shear transformation zone plasticity**

A Benzerga, B Kondori and A Needleman

Texas A&M University, USA

A computational method for solving small strain plasticity problems with plastic deformation arising from the evolution of a collection of discrete shear transformation zones (STZs) is presented. The STZs are represented as transforming Eshelby inclusions. At each instant, superposition is used to represent the solution in terms of the Eshelby inclusions, which are given analytically for an infinite elastic medium, and an image solution that enforces the prescribed boundary conditions on the finite body of interest. The image problem corresponds to a standard linear elastic boundary value problem. Constitutive relations are specified for the kinetics of the transformation. The general three-dimensional formulation is given. Solutions for compression of a plane strain block are presented that illustrate the potential of the framework.

Symposium E

(E1 invited) **Multiscale modeling of coherent precipitation in interstitial solid solutions**

M Asta, D Olmsted and M de Jong

University of California, Berkeley, USA

In many technologically important structural alloys, coherent precipitation plays an important role in governing mechanical behavior. The formation of small coherent precipitates can be advantageous, as in the case of strengthening of Al alloys, or deleterious, as in the embrittlement of hcp Ti. In both cases, computational modeling of solvus boundaries and related thermodynamic properties relevant to nucleation and coarsening is challenged by the need to model elastic and chemical contributions to the free energy on the same level. In this talk we describe the application of a mixed-basis cluster expansion approach based on density-functional theory (DFT) in the context of modeling coherent oxide precipitates in hcp-Ti. Our approach employs lattice Green functions and Kanzaki force models computed from first-principles DFT calculations, to model long-ranged strain-mediated solute interactions. The elastic-energy model is combined with the DFT-parameterized cluster-expansion formalism for modeling interactions on short to medium range scales. We demonstrate the application of this approach in the context of Monte-Carlo based modeling of coherent phase boundaries and precipitate morphologies in hcp Ti(O) solid solutions.

(E1 oral) **Nb precipitation in zirconium alloys**

M Cottura and E Clouet

SRMP - CEA Saclay, France

Precipitates are very effective in strengthening metallic alloys because they can act as obstacles to dislocation motion. One of the key factors that controls the mechanical properties of precipitate-hardened alloys is the morphology of the precipitates i.e. their size and shape. In Nb-containing zirconium alloys, currently employed in nuclear power plants, niobium precipitation occurs under irradiation. Coherent β-Nb nano-precipitates (bcc structure) presenting a platelet shape lying in the basal plane appear in the α-Zr matrix (hcp). The purpose of the present work is to investigate the different factors that might control the precipitate morphology, i.e. the interfacial and elastic strain energies.

First, an *ab initio* study of coherent Zr/Nb interfaces has been carried out to evaluate the anisotropy of the interface energies. The favoured interfaces are compared to interfaces evidenced by high resolution electron microscopy. Then, the elastic energy for the Zr/Nb system has been determined from the continuous inhomogeneous and anisotropic elasticity theory. The results obtained will give us the necessary energetic information's to predict the equilibrium morphology of the β-Nb precipitates as a function of size. A comparison with experimental observations will be done to assess deviations from the equilibrium shape.

(E1 oral) **Multiscale modelling of Ti-Al-N thin film growth using DFT and kMC approaches: microstructural evolution**

C Mastail, F Nita, M David, A Michel and G Abadias

Institut Pprime, France

Transition metal nitride (TMN) exhibits a unique combination of metallic, ionic and covalent bonding exploited in semiconductors, a refractory character resulting in high hardness, chemical inertness and thermal stability, which makes them used as protective and wear-resistant coatings. Depending on the deposition conditions, ternary TMN thin films may be synthesized with different structural properties: bi-phase nanocomposite or metastable cubic solid solution. The elastic properties and ductility trends in polycrystalline TMN were shown to be affected by the microstructure and preferred orientation, which can vary significantly with film thickness and alloy composition.

Predictive design of these materials can be achieved by using multi-scale computational approaches to mimic real deposition conditions and gain insights on thin film evolutions during growth. The accurate description of growth kinetics and energetics remains a challenging task, especially for magnetron sputtering for which particle bombardment may alter the resulting microstructures.

To predict the microstructure and morphology evolution during sputter-deposition of ternary TiAlN films, we have performed kinetic Monte Carlo (kMC) simulations using a 3D rigid lattice model. The lattice is obtained by a superposition of two FCC sub-lattices, each of them corresponding to a kind of atom (metal sub-lattice and N sub-lattice). For both kinds of particles, two main events are considered, 3D diffusion and deposition. Activation energy barriers for diffusion have been computed by DFT, using either existing literature values or from the present work. The influence of main growth parameters (growth rate, temperature, working pressure, stoichiometry) on the resulting microstructure will be presented and discussed.

(E1 oral) **Effect of interfacial structure on the heterogeneous nucleation of Pb at a Cu surface**

B Laird and P Palafox-Hernandez

University of Kanas, USA

In previous simulation studies using embedded atom potentials of the chemically heterogeneous solid-liquid interface of Pb(*l*) at a Cu(*s*) surface [1], we reported a strong dependence of the interfacial structure on interface orientation. For the Cu[100]/Pb(*l*) interface, significant surface alloying was observed. However, for the Cu[111]/Pb(*l*) solid-liquid interface, no alloying was seen, instead the system exhibits "prefreezing" in which the first few layers of Pb are crystalline at temperatures just above the Pb melting point (618K for this model of Pb), with a 2-d hexagonal structure that is rotated by 6° relative to the underlying Cu lattice. This prefreezing layer is atypical in that the width of the layer does not diverge as the system is cooled towards the Pb melting temperature. In this work, we examine the effect of the interfacial structure on the orientation dependence of the heterogeneous nucleation rates for undercooled Pb(*l*) at a Cu surface. Heterogeneous nucleation is seen to occur readily at the Cu[111] surface on the molecular-dynamics (MD) simulation time scale at temperatures near 590K; however, for the Cu[100] surface, the Pb will only solidify on the MD time scale for temperatures that are considerable lower - around 450K. This indicates that the presence of the prefreezing layer considerably lowers the barrier to heterogeneous nucleation of Pb at a Cu substrate. Estimates of the nucleation rates and activation energies will be reported as well as detailed structural information about the nucleating cluster.

[1] Acta Mater. 59, 3137 (2011)

(E2 invited) **Combination of atomistic simulation and phase-field modelling techniques for a texture control in steel sheets**

B-J Lee and K-M Kim

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Phase-Field models provide the best simulation tool for the effect of grain boundary (GB) or surface segregation of impurity atoms on microstructural evolution. Today, fundamental materials information such as the amount of solute segregation and resultant reduction of GB or surface energy can be provided by atomistic simulation techniques in a functional form of the orientation of GBs or surfaces. However, it looks difficult to reproduce the amount of solute segregation and resultant reduction of GB or surface energy, simultaneously, using the existing Phase-Field models.

In the present talk, a multiscale computational approach to develop highly value-added {100} textured steel sheets will be briefly outlined. Some technical difficulties met during the Phase-Field modelling and simulation, and the ways to avoid the difficulties will also be introduced.

(E2 oral) **Simulation and modelling of electromigration of C in Fe: a molecular dynamics approach**

P Chantrenne[1], Q Rong[1], B Yeroshenko[1], O Waseda[1], J Amodeo[2], R Veiga[3] and M Perez[1]

[1]INSA, France, [2]University Sao Paulo, Brazil

Electromigration is a diffusion-based phenomenon leading to the anisotropic migration of metallic species under an electric field. It occurs for example at electric connectors interfaces creating short circuit or circuit opening. In bulk materials, this phenomenon also induces chemical concentration gradients and thus modifying the microstructure and other physical properties. Despite its importance in the field of electronics and other applications, there is a lack of knowledge and understanding on electromigration in alloys, especially for quantification and measurement methods where only few studies dedicated to aluminium alloys and steels have already been published. From a theoretical point of view, the Nernst Einstein model predicts the drift velocity induced by electromigration, but does not explain non linearity between the drift velocity and electric field. In this study, we propose a new theory to predict drift velocity applied to the Fe-C system, where material properties such as diffusion coefficient, energy barrier and C vibration frequencies are determined using atomistic simulations.

For the atomistic simulations, a new combination of interatomic potentials is used: the Meyer potential which describes the Fe-Fe interaction of ferrite and austenite and the Becquart potential for the Fe-C interaction. Despite the C diffusion coefficient and the Fe defect structural properties might not be realistic, this combination allows studying the Fe a-g phase transformation induced by C diffusion.

The drift velocities obtained with MD and the new model are in good agreement. This methodology developed for a Fe-C system might then be used for different kind of systems.

(E2 oral) **A molecular dynamics study of the effect of helium clusters on grain boundary migration in bcc iron**

A T Wicaksono, M Militzer and C Sinclair

University of British Columbia, Canada

Models on the kinetic interaction between grain boundaries and impurities can be grouped into two categories based on the size and the mobility of impurities. Solute drag models consider the effect of ideal solute atoms on a migrating boundary, where the drag pressure has a non-linear dependence on the boundary velocity. Particle pinning models, on the other hand, account for the restraining effect of stationary precipitates on the boundary migration that is independent of the velocity.

Impurities that form clusters correspond to an intermediate case because clusters do not exhibit a packing order as distinct as that of particles and have lower diffusivities than solute atoms. The cluster-boundary interaction, however, has not been fully explored despite its technologically important roles, e.g. embrittlement of irradiated steel reactors due to helium (He) clusters

In this work, the interplay between He segregation, He cluster formation and curvature-driven boundary migration in BCC iron (Fe) has been investigated using molecular dynamics simulations. He atoms that segregate to the migrating boundary are found to be trapped in the vacant substitutional sites emitted by the boundary. He atoms that form clusters in the bulk restrain the migration via a pinning mechanism, where the cluster pinning is proportional to the density and the squared radius of each cluster. A cluster pinning model has been developed by incorporating the twofold effect of clusters on the boundary migration: (1) reducing the boundary mobility and (2) acting as pinning objects that delay or even completely halt the migration.

(E2 oral) **Multi-scale study of the gas-phase growth of Silicon clusters in realistic conditions**

G Barcaro[1], S Monti[2], L Sementa[1] and V Carravetta[1]

[1]CNR-IPCF (Italian National Research Council, Institute for Physical and Chemical Processes), Italy, [2]CNR-ICCOM (Italian National Research Council, Institute for Organometallic Complexes), Italy

Bottom-up synthesis by gas-phase processes has a remarkable technological interest because it can produce dry and thermally-stable crystalline nanoparticles in a single step. In this perspective, the availability of a multi-scale approach to study gas-phase growth is mandatory to achieve a deeper comprehension of the nucleation and growth processes, which can furnish important information to orient the synthesis techniques towards an optimization of the growth protocol. These topics are the subject of a recently granted project, NanoDome, which has received funding from the European Union's Horizon 2020 Research and Innovation Programme, under Grant Agreement n. 646121.

Within the present study, we will show the results of an atomistic study concerning the nucleation and the growth processes of Silicon clusters generated in plasma conditions (very high temperature ranging from 1000 to 5000 K) in presence of buffer gases (both unreactive, like Argon, or reactive, like Hydrogen and Nitrogen) by taking advantage of a joint protocol of ab-initio calculations (at both zero and finite temperature) and classical molecular dynamics using Reactive Force Fields. The correct parametrization at the first-principles level of all the inter-atomic potentials has allowed the investigation of the growth process covering a size range where first-principles dynamics cannot be performed. From these latter simulations it is possible to extract important information to feed mesoscale models towards a real multi-scale protocol aimed to a full description of the evolution of the nanoparticle population from the embryo atomic-cluster appearance to the formation and dynamics of nanoparticle aggregates.

(E2 oral) **Multiscale simulation of interface-dominated structural transformations in Fe-C alloys**

X Zhang[1], T Hickel[1], J Rogal[2], R Drautz[2] and J Neugebauer[1]

[1]Max-Planck-Institut für Eisenforschung, Germany, [2]Ruhr-Universität Bochum, Germany

The microstructure evolution in structural materials is often controlled by structural phase transformations at dynamic interfaces. For instance, a classical lamellar microstructure in steels named pearlite originates from the structural decomposition of a face-centered cubic (fcc) austenitic phase into a body-centered cubic (bcc) ferritic phase and an orthorhombic carbide, cementite (Fe_3C) at the interface. Since the relevant mechanism consists of a set of simultaneous structural transformations and of various interfaces, a direct *ab initio* modelling of such a microstructure is computationally too expensive. Hence, in this work, we propose a multiscale approach that simulates this type of microstructure by treating the bulk structural transformations with *ab initio* nudged elastic band methods and considering the interfaces as constraints applied on the transformations. Using this approach, we are able to capture the different atomistic mechanisms for the structural transformations among the three phases depending on the local conditions (magnetism, strain and C concentration) that are enforced by the specific interfaces. The formalism developed here is general and can be applied to other material systems and microstructures.

(E3 invited) **Microstructural pattern formation during liquid metal dealloying**

A Karma[1], P-A Geslin[2], I McCue[3] and J Erlebacher[3]

[1]Northeastern University, USA, [2]Claude Bernard University Lyon, France, [3]Johns Hopkins University, USA

Liquid metal dealloying (LMD) has emerged as a novel technique to produce topologically complex nanoporous and nanocomposite structures with ultra-high interfacial area and other unique properties relevant for diverse materials applications, exemplified by Si for battery anodes with extremely long cycle fatigue, nonporous Nb for electrolytic capacitors, or Cu-Ta nanocomposites with outstanding material properties. LMD offers similar advantages as the traditional electrochemical dealloying method for forming desirable structures, but is applicable to a larger class of materials by using a liquid metal instead of an acid bath as conduit for the selective dissolution of one element of a multicomponent alloy. How dealloyed structures form has remained somewhat of a mystery. I will discuss the results of a recent study that combines phase-field simulations, experiments, and theoretical analysis to unlock this mystery. Simulations and experimental observations reveal how diffusion-limited interfacial and bulk transport phenomena interact to form a rich variety of topologically disconnected and connected structures. Moreover, analysis of the results yields scaling laws governing nano/microstructural lengthscales and dealloying kinetics that provide a quantitative theoretical basis for controlling dealloyed structures.

(E3 oral) **Diffuse interface modelling of microstructure evolution in the presence of flow: Hydrodynamics equations**

F Varnik, A Subhedar and I Steinbach

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Adequate modelling of hydrodynamic transport is of key importance for solidification and microstructure evolution [1]. In view of the wide spread use of diffuse interface approaches such as the phase field method, we focus here on modelling hydrodynamic equations in the presence of a diffuse solid-liquid interface via a volume averaging approach [2]. The resulting equations exhibit the same structure as the standard Navier-Stokes equation for a Newtonian fluid with a constant viscosity, the effect of the solid phase fraction appearing in the drag force only [3]. This considerably simplifies the use of the lattice Boltzmann method as a fluid dynamics solver in solidification simulations. Galilean invariance is also satisfied within the new approach. Further, we investigate deviations between the diffuse and sharp interface flow profiles via both quasi exact numerical integration and lattice Boltzmann simulations. It emerges from these studies that the freedom in choosing the solid-liquid coupling parameter, h, provides a flexible way of optimizing the diffuse interface-flow simulations. Once h is adapted for a given spatial resolution, the simulated flow profiles reach an accuracy comparable to quasi exact numerical simulations [3].

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[2] D. A. Drew, Mathematical Modeling of Two-Phase Flow, Annual Review of Fluid Mechanics 15, 261 (1983)
[3] A. Subhedar, I. Steinbach, F. Varnik, Modelling the flow in diffuse interface methods of solidification, Phys. Rev. E 92, 023303 (2015)

(E3 oral) **Modeling pattern formation in multi-component fluids on the mescoscale: a phase-field approach**

G Toth and B Kvamme

University of Bergen, Norway

A generalization of the Cahn-Hilliard theory of binary liquids is presented for multicomponent incompressible liquid mixtures. First, a thermodynamically consistent convection-diffusion-type dynamics is derived on the basis of the Lagrange multiplier formalism. Next, a generalization of the binary Cahn-Hilliard free-energy functional is presented for an arbitrary number of components, offering the utilization of independent pairwise equilibrium interfacial properties. We show that the equilibrium two-component interfaces minimize the functional, and we demonstrate that the energy penalization for multicomponent states increases strictly monotonously as a function of the number of components being present. We validate the model via equilibrium contact angle calculations in ternary and quaternary (four-component) systems. Simulations addressing fluid flow-assisted spinodal decomposition and emulsion formation in these systems are also presented. The proposed approach opens the possibility of designing structured multi-component fluids, such as templating materials, bi- and tricontinuous polymer mixtures, etc. used in many applications, including advanced drug delivery or effective CO2 storage.

(E3 oral) **Metal droplet entrainment by solid particles in slags: a combined phase field – experimental approach**

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Various pyrometallurgical industries encounter production losses due to the mechanical entrainment of metallic droplets, i.e. the droplets are attached to solid particles in liquid slags. The attached metal cannot settle, decreasing the yield of the phase separation. This results in inadequate sedimentation and eventually production losses in e.g. industrial Cu smelters and Pb reduction melting furnaces.

Experimental work on this topic started recently but remains challenging. Phase field simulations can circumvent this lack of experimental data and allow a more systematic evaluation on the role of different parameters on the observed phenomenon. However, simulations are best interpreted in combination with experiments. The performed experiments are used both for the input microstructure of the solid particles and to validate the simulation results.

A binary phase-field model simulates the attachment of liquid metal droplets to solid particles in slags and considers realistic microstructures of solid particles in slags. Furthermore, two initialization methods for the liquid metal droplets are compared. Both initializations correspond well with experimental observations, which points to the existence of several origins for the attachment of metal droplets to solid particles in slags. One initialization corresponds to a case where the droplets are formed by a chemical reaction in which both the droplets and the spinel solids are involved. The other initialization corresponds to a situation where the droplets and particles are formed separately and independently and are then mixed in the slag.

(E4 invited) **Multiscale modelling of structure evolution in industrial materials**

J Ågren

KTH, Sweden

Modelling of structural evolution during synthesis, processing and usage of materials is a key element in Materials Design based on ICME (integrated computational materials engineering) and the materials genome. The centre Hero-m, hosted at KTH, was launched 2007 as a long-term collaborative effort between Swedish industry, an industrial research institute and KTH. Hero-m has the mission to develop tools and competence for fast, intelligent and cost efficient product development for Swedish industry and its activities are based on ICME and multiscale modelling. Some general aspects of materials design, ICME and the materials genome will be discussed. Some examples where modelling of structural evolution using a combination of DFT and experimental information in the CALPHAD genomic language will be presented. These involve high-performance steels as well as hard metals based on cemented carbides.

(E4 oral) **Modelling microstructure evolution in metallic alloys: elasticity and plasticity**

Y Le Bouar[1], M Cottura[2], P-L Valdenaire[3], B Appolaire[3] and A Finel[3]

[1]CNRS/ONERA, France, [2]SRMP, CEA, France, [3]LEM, CNRS/ONERA, France

Many materials used in everyday life have a complex internal structure organized at different scales with a texture of grains, and a complex pattern of thermodynamic phases at lower scale. This microstructure strongly impacts the movement of crystalline defects in the materials and therefore controls the mechanical behaviour. The phase field method has emerged as the most powerful method for tackling microstructure evolutions during phase transformations when elastic coherency stresses are generated. In addition, in many materials and especially at high temperature, the microstructure evolution is coupled with plasticity, and there is currently a great research effort to extend the phase field method to take this coupling into account.

In this context, I will first present a new multi-grid spectral scheme to solve elastic equilibrium in an elastically heterogeneous and anisotropic medium. Then, I will show how to couple a classical phase field model (for the description of the phase transformation) with a crystal plasticity model based on dislocation densities. The latter model uses a storage-recovery law for the dislocation density of each glide system and a hardening matrix to account for the short-range interactions between dislocations. The proposed model will be first applied to simple microstructures to illustrate the importance of the size effect and of the anisotropy of plasticity in heterogeneous materials. Finally, the coupled model will be applied to study rafting of ordered precipitates observed in Ni-based superalloys during creep.

(E4 oral) **Optimize material parameters with 4D experiments and phase-field simulations**

J Zhang[1], S Poulsen[2], P Voorhees[2] and H Poulsen[3]

[1]Technical University of Denmark (DTU), Denmark, [2]Northwestern University, USA

In this paper, we propose a new way to determine material parameters by comparison between 4D experiments and phase-field simulations. The evolution of the material microstructure is measured using in situ X-ray tomographic microscopy. Using the first frame from the experiment as input, the evolution of the material microstructure is simulated using the phase-field model. An iterative optimization technique is used to find the material parameters that yield the best match of the simulated microstructure to the measured microstructure in a global manner. The proposed method is applied to a hypo-eutectic Al-Cu system to determine the liquid diffusion coefficient.

(E4 oral) **Effects of fcc/fcc grain boundaries on the formation of bcc phase in pure iron by molecular dynamics simulation**

X Ou, J Sietsma and M J Santofimia

Delft University of Technology, Netherlands

Molecular dynamics simulations were used to study the effects of three different fcc/fcc grain boundaries, with different misorientations, on the nucleation and growth of bcc phase in pure iron. The studied fcc/fcc grain boundaries were: one low-angle grain boundary (LAGB), one high-angle grain boundary (HAGB) and one coherent twinning boundary. The LAGB and the HAGB were constructed by rotating part of a single fcc crystal by about 5° and 45° around the $[0\ 1\ 0]_{fcc}$ direction, respectively. The LAGB is semi-coherent with periodic dislocations, while the HAGB is incoherent. Heterogeneous nucleation of bcc phase was found to take place at both the LAGB and the HAGB, whereas homogeneous nucleation was not observed. The nuclei forming at the coherent part of the LAGB shows a Kurdjumov-Sachs (KS) orientation relationship with both parent fcc crystals. The nuclei forming at the incoherent part of the LAGB or at the HAGB has a special orientation relationship with one of the parent fcc crystals, either in the Pitsch Orientation or the KS orientation. No phase transformation was observed for the coherent twinning boundary after a simulation time of 100 ps. It was estimated that the newly formed bcc/fcc interfaces propagated into the original fcc phase at an velocity on the order of 1000 m/s, which exhibits a martensitic nature.

(E5 invited) **The role of the mesoscale in grain boundary migration**

C Race[1], R Hadian[2], B Grabowski[2] and J Neugebauer[2]

[1]University of Manchester, UK, [2]Max Planck Institut fuer Eisenforschung, Germany

We have studied the velocity, morphology, and mechanisms of moving grain boundaries below the roughening temperature using molecular dynamics simulations. When the area of the grain boundary is small or the simulation is quasi-two-dimensional (as it often is in simulations) the boundary moves via the coordinated rearrangement of the crystal at the boundary. However, in more realistic simulations, when the boundary has a larger area, its motion requires the formation of "islands" of reoriented crystal bounded by disconnections. We show that the kinetics of this homogeneous nucleation process provide a quantitatively accurate prediction of the complicated driving-force-dependent and temperature-dependent behaviour that emerges from our simulations. As a consequence, it is no longer possible to identify a driving-force-independent activation energy for grain boundary migration and the concept of an intrinsic mobility for smooth boundaries is thus inappropriate.

We further show that the presence of certain types of defects in a grain boundary surface removes the need for homogeneous nucleation. The migration kinetics of such defective boundaries agree with the expected picture of a mobility independent of driving force. This mobility is now, however, a function of the defect content and morphology of the boundary rather than a property of the boundary geometry alone.

(E5 oral) **Linking design of materials and technological process parameters for tailored integration in microelectronics field: climbing the scales**

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New advanced nanoscale-controlled materials could offer unique functionalities in various areas such as the ultrathin films in nanotechnology. Increasing our knowledge and understanding of properties of directly integrated materials at an atomistic level and developing the means of predicting and controlling their structures and functions at the nanometre scale will help to push forward their tailored elaboration. Understanding how matter organizes at the atomic scale during deposition of ultrathin materials in close relation with elaboration process parameters is the addressed topic.

It is then necessary to use simulation methods with different length and time scales in order to get a precise description of the physics and chemistry of phenomena but also an overlook on the growth of materials. In our approach, we propose a multilevel approach where modelling / simulation tools are used as a bottom up strategy from atomic scale to simulation platform development linking design and manufacturing. We propose a model based on a kinetic Monte Carlo (KMC) method to simulate growth of directly integrated materials to understand and evaluate the influence of experimental conditions on the nanostructuring and final performances of integrated nanomaterials with the aim to improve their integration into devices. Illustrations on growth of oxide layers under technological processes will be given, notably SiO2 growth through thermal oxidation and CuO growth on Al surface through PVD.

(E5 oral) **Size-effects on grain growth by MD-simulations**

P W Hoffrogge and L Barrales-Mora

IMM, Germany

It is well known that different physical mechanisms are activated in nanostructured materials owing to the size of the crystallites that inhibits mechanisms present at larger sizes. This phenomenon is usually referred to as a size-effect. The present contribution was motivated to elucidate possible size-effects on grain growth of nanostructured materials. For this purpose, we developed an algorithm that allows determining the relative orientation of atoms in molecular dynamics simulations. The method can be utilized to resolve grains in polycrystalline ensembles, to track the evolution of individual grains and to study separately mechanisms for grain growth. The algorithm was utilized to study grain growth in three polycrystals with different initial grain sizes but otherwise with crystallographically equal and isomorphic grains.

(E5 oral) **Influence of precipitation kinetics on static recrystallization during hot deformation of a 2xxx aluminium alloy**

E Kabliman, S Bozorgi, I Baumgartner and J Kronsteiner

LKR Leichtmetallkompetenzzentrum Ranshofen GmbH, Austria

Ultrafine grained metals produced by severe plastic deformations to high strains often have high strength, but poor ductility limits their practical application. Introduction of recrystallized grains into the nanocrystalline matrix to create a 'composite' structure has been suggested as an approach to improve ductility of such materials. However, the amount of recrystallized grains needed for improving ductility varies significantly for different samples, which may be related to the local strain distributions during deformation. In this work, we studied two partially recrystallized high purity copper samples using in-situ tensile tests: 1) a sample cold rolled to a strain of 2.3 and annealed and 2) a sample deformed by dynamic plastic deformation to a strain of 2.1 and annealed. Both samples contain around 50% volume fraction of recrystallized grains. Changes in the microstructures during in-situ straining were characterized by both backscattered imaging and electron backscatter diffraction (EBSD). The local strain distributions in different recrystallized grains and in the remaining non-recrystallized matrix were quantified using digital image correlation (DIC). The strains determined using DIC were compared with the misorientations determined from EBSD. Crystal plasticity modelling was also applied for comparison.

(E6 invited) **Growth and ripening under mechanochemical coupling**

R D Kamachali, C Schwarze and I Steinbach

ICAMS - Ruhr-Uni-Bochum, Germany

The diffusion-controlled growth and ripening of precipitates are well studied in many aging materials. The challenge, however, remains unfinished to encounter simultaneous chemical and elastic effects with cross-coupling between them as demonstrated recently [1, 2]. Theoretical derivations and mesoscale phase-field simulations of growth and ripening in shape memory alloys and Al systems are performed to take these effects into account. Kinetics and statistical analysis are conducted to understand the effect of elasticity and mechanochemical coupling. The results show that the growth generally slows down at the presence of elasticity and coupling. Inverse ripening at the presence the mechanochemical effect is observed.

[1] R. Darvishi Kamachali, E. Borukhovich, N. Hatcher and I Steinbach; "DFT-supported phase-field study on the effect of mechanically driven fluxes in Ni4 Ti3 precipitation"; MSMSE 22 (2014) 034003

[2] R. Darvishi Kamachali, E. Borukhovich, O. Shchyglo and I. Steinbach; "Solutal gradients in strained equilibrium"; Phil. Mag. Let. 93 (2014) 680

(E6 oral) **Ab initio study of the influence of hydrogen and iron on the nucleation of prismatic loops in Zr alloys submitted to irradiation**

B Christiaen[1,2,3], A Legris[2,3], C Domain[1,2], L Thuinet[2,3] and A Ambard[1,2]

[1]EDF-R&D, France, [2] EDF-CNRS Etude et Modélisation des Microstructures pour le Vieillissement des Matériaux (EM2VM), France, [3]Unité Matériaux Et Transformations, UMET, UMR 8207, ENSCL, Université Lille 1, France

Zirconium alloys are used to manufacture fuel cladding as well as fuel assembly. Under irradiation, they show a dimensional change commonly called growth. Recrystallized alloys are used for guide tubes. Experimental observations have shown that above a threshold dose those alloys are prone to an accelerated growth called “breakaway”. It has been well established that dislocation loops <a> and <c> are directly responsible for the growth of zirconium alloys under irradiation and that <c> loops are correlated with breakaway. However, the nucleation mechanisms in which alloying elements are known to play an important role are still poorly understood. In order to improve our understanding, calculations based on density functional theory (DFT) are used to simulate point defect clusters with different geometries. The effect of alloying elements such as iron and hydrogen as well as the topology of the various simulated objects on their thermodynamic stability is discussed.

(E6 oral) **Modelling recrystallization and massive α/γ transformation during intercritical heating of a Dual Phase steel**

M Ollat[1], M Perez[1], V Massardier[1], D Fabregue[1] and E Buscarlet[2]

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Massive ferrite to austenite transformation is a key process in the steel industry. In order to optimize heating rate and austenitizing time and temperature, a modelling approach is proposed in this paper. As recrystallization strongly influences the kinetics of the massive transformation on cold rolled steels, a coupled approach was developed accounting for the recrystallization and the α→γ transformation. The recrystallization model is based on JMAK formalism. The massive transformation model is based on the diffusion limited interface migration. Both models are calibrated using isothermal experiments and their coupled predictions are successfully compared to non-isothermal experiments.

(E6 oral) **Phase field modelling of abnormal grain growth**

Y Liu[1], M Militzer[1] and M Perez[2]

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Heterogeneous grain structures may develop due to abnormal grain growth during processing of polycrystalline materials ranging from metals to ceramics. The phenomenon must be controlled in practical applications where typically homogeneous grain structures are desired. Recent advances in experimental and computational techniques have, thus, stimulated to revisit the underlying growth mechanisms. Here, phase field modelling is used to systematically evaluate conditions for abnormal grain growth. Grain boundaries are classified into two classes, i.e. high and low mobility boundaries. Three different approaches are considered for having high and low mobility boundaries: (i) critical threshold angle of grain boundary disorientation above which boundaries are highly mobile, (ii, iii) two grain types A and B with either the AA or the AB boundaries being highly mobile. For these different scenarios 2D and 3D simulations have been performed to quantify the effect of variations in the mobility ratio, threshold angle and fractions of grain types, respectively, on the potential onset of abnormal grain growth and the degree of heterogeneity in the resulting grain structures. The required mobility ratios to observe abnormal grain growth are quantified as a function of the fraction of high mobility boundaries. The mechanisms of abnormal grain growth are analyzed in terms of the spatial distribution of the high mobility boundaries.

(B1+E7 invited) **Strategies and algorithms for the automated parallel data mining of annealing microstructure evolution pathways**

M Kühbach, C Miessen, L A Barrales-Mora and G Gottstein

RWTH Aachen University, Germany

One gap in our current understanding of annealing microstructures is the significance of structural heterogeneities and spatial property correlations for the growth of individual grains. A solution is seen in the combination of detailed 3D resolved in-situ experiments and the parallelized computer modeling and simulation of statistical significant model microstructures. It is expected that both methods will continue to grow in numerical capacity and impact in the next years.

However, one key question to these methods, and time-resolved 3D simulations in particular, is how they can be practically processed and screened in an automatized manner, such as to identify grains with significant effect on the evolution of the grain boundary network.

We present one solution strategy which is to post-process instrumented computer simulations in 3D with parallelized data mining algorithms. Specifically, we aim to extract the growth paths of individual grains and to relate these to their topological activity, orientation and neighbourhood. In combination with very large synthetic microstructures, this enables us to gather statistics of the rare events during phenomena such as abnormal grain growth or the preferential evolution of particular subgrains during discontinuous recrystallization.

(B1+E7 oral) **Coupled microstructural and mechanical models for non-isothermal treatments of a 6061 aluminum alloy**

D Bardel, T Chaise, M Perez and D Nelias

INSA Lyon, France

In age-hardening alloys, high-temperature processes, such as welding, can strongly modify the precipitation state, and thus degrade the associated mechanical properties. The aim of this contribution is to present a coupled approach able to describe precipitation, associated yield stresses and kinematic/isotropic hardening for non-isothermal treatments of a 6061 aluminium alloy. A thermomechanical machine has been specially designed to perform fast and controlled non-isothermal cycles representative of different positions along the weld.

The precipitation state (in terms of volume fraction and precipitate size distribution) is modelled thanks to a recent implementation of the classical nucleation and growth theories for needle-shaped precipitates (see Bardel et al, Acta Mater. (62), 2014).

The precipitation model is validated through Small-Angle Neutron Scattering (SANS) and Transmission Electron Microscopy (TEM) experiments. The precipitation size distribution is then used as an entry parameter of a micromechanical model for the yield strength and kinematic/isotropic hardening of the alloy (see Bardel et al, Acta Mater. (83), 2015).

Predicted stress/strain curves are compared to tensile cyclic tests performed with various heating conditions, representative of the heat-affected zone of a welded joint.

(E8 invited) **Multiscale modeling of the recrystallization**

M Bernacki, N Bozzolo, C Moussa and D P Muñoz

Mines ParisTech, France

The mechanical and thermal properties of metallic materials are strongly related to their microstructure. The understanding and modeling of the mechanisms governing the microstructural evolutions is then crucial when it comes to optimize the forming process and the final in-use properties of the materials.

To treat in an average way, the evolution of the material microstructure during thermal and mechanical treatments, the classical method, well known as “mean field” approach, consists in fact in a macro description, selecting representative material parameters (grain size, inclusions, phase percentage, precipitates…) and identifying physical laws which govern the evolution of these parameters, and their influence on the mechanical behaviour.

On the other hand, computation at the mesoscale is now possible and is developed for a potentially more realistic description of materials under the concept of “full field” approach. For example, recently, a new full field model using the level set method in a finite element framework has been proposed. The latter enables to model 2D and 3D recrystallization by describing the polycrystalline microstructure, including the nucleation stage and has been extended to take into account the grain growth stage.

The interests of these precise approaches lie in the possibility to predict non averageable phenomena but also to discuss/optimize/propose custom-made mean field models.

An illustration of this multiscale approach applied on 304L stainless steel will be detailed.

(E8 oral) **Simulation of sub-grain growth utilizing a computationally efficient level-set model**

C Mießen, M Kühbach, N Velinov, L Barrales-Mora and G Gottstein

RWTH Aachen University, Germany

In our contribution, we present a new implementation strategy for level-set algorithms to grain growth in two and three dimensions. Our model is capable of considering the full complexity of the grain boundary properties such as energy and mobility depending on misorientation. We present recent developments on the level-set approach to grain growth, considering technical improvements to include anisotropies of different microstructural elements in three dimensions and advanced implementation strategies for modern parallel computer architectures. To benefit from these systems, the original microstructure was decomposed into grains to achieve a homogeneous distribution of the computational tasks. This object based approach permits to track the evolution of individual grains, as well as their topological paths. We utilized the model to simulate sub-grain growth in a microstructure with different orientation bands after 70% cold-rolled aluminum. Data mining techniques were utilized subsequently to analyse the topological paths of grains and their relationship to their short- and long-range environment.

(E8 oral) **Investigation of nanoscale field emitters on copper surfaces under high electric field**

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[1]University of Tartu, Estonia, [2]University of Helsinki, Finland

Localized enhancement of the electric field near metal surfaces is a significant factor in high-electric field applications, such as particle accelerators. For example, the Compact Linear Collider (CLIC), a new particle accelerator planned at CERN, uses surface electric fields up to 300 MV/m. The accelerating electric field can be further enhanced by localized surface defects, ultimately leading to electrical breakdowns in Cu accelerating structures. Localized field enhancement is presumably caused by nanoscale field emitters, spontaneously appearing on the surface during normal operation of accelerating structures.

We combine Finite Element Analysis, molecular dynamics, and Hybrid Electrodynamics Molecular Dynamics code HELMOD to investigate electrical, thermal and mechanical behaviour of material surface, influence of nanoscale surface protrusions and possible mechanisms leading to the formation of such surface defects. Both electrical and thermal simulations account for nanoscale size effects. The simulation of emission currents covers field and thermal emission, while the temperature balance of the material is simulated using Joule heating and contribution from the Nottingham effect. The mechanical behaviour of the material is mainly covered by molecular dynamics calculations, with FEA extending the studies of elastic and plastic deformations towards microscale.

It is found that possible changes in the current emission regimes can lead to significant differences in estimated field enhancement factor values. Moreover, strong electric fields, applied to the Cu surface can have both, stabilizing and destabilizing effects on the protrusions, providing a possible mechanism to explain the lack experimentally observable nanoscale field emitters on Cu surfaces.

(E8 oral) **Comparison of dislocation-based model of recovery and cross-correlation based EBSD measurements in single crystals**

S Kalácska, P D Ispánovity and I Groma

Eötvös Loránd University (ELTE), Hungary

Subgrain growth during recovery has been investigated using simulations of two-dimensional discrete dislocation dynamics on a hexagonal lattice having three symmetric slip planes [1]. To account for elevated temperature (i) dislocation climb was allowed and (ii) a Langevin type thermal noise was added to the force acting on the dislocations. The growth exponent and the subgrain structure were examined.

Cross-correlation based analysis of electron backscatter diffraction (EBSD) patterns is often carried out to map plastic strain variations in deformed polycrystalline samples [2]. Firstly, the effects of sample surface preparation methods were investigated including Ar ion polishing and traditional electropolishing treatments. Then the distortion maps of the specimen are computed with the cross-correlation technique. This method is capable of detecting changes of the crystal orientation to higher accuracy, than the commercial software provided for standard EBSD devices that analyse each EBSD pattern individually.

In this work the simulation and experimental results were compared to characterize the evolution of dislocation structures and corresponding distortion fields in highly deformed Cu single crystals during low temperature annealing.

[1] P.D. Ispánovity, I. Groma, W. Hoffelner and M. Samaras, Abnormal subgrain growth in dislocation-based model of recovery. Mod. Simul. Mat. Sci. Eng. 19 (2011) 045008

[2] Britton and A.J. Wilkinson, High resolution electron backscatter diffraction measurements of elastic strain variations in the presence of larger lattice rotations. Ultramicroscopy 114 (2012) 82-95

(E9 invited) **Plasticity at the microscale: a discrete dislocation dynamics study of the role of interfaces and strain gradients on the effective plastic slip distribution**

D Weygand and M Stricker

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The mechanical behaviour of micrometre sized specimens is directly controlled by the microstructure comprising both dislocation structure and interfaces. These are natural obstacles to dislocation glide leading to pile-up formation and the development of plastic strain gradients. Discrete dislocation dynamics simulations of multigrain aggregates show, that the elastic interaction between dislocations of different grains change the plastic strain profile close to the grain boundaries significantly, even though the grain boundary is acting as an obstacle [1,2]. This intrinsic behaviour is lacking in continuum descriptions.

To explore further the role of gradients due to external boundary constraints, a comparative analysis of torsion simulations using discrete dislocations, extending the preliminary work of Senger et al. [3], and standard crystal plasticity is presented. The discrete dislocation dynamics show complex dislocation entanglements which lead to unexpected strain distributions, when compared to current continuum descriptions. These findings are discussed with respect to the question of volume averaging of discrete dislocation results, development of internal stresses due to gradients and the influence of crystal orientation on the formation of extended plastic slip. These information's may provide important insight for improving dislocation density based continuum theories, which should be able to capture dislocation both the transport of dislocations and hardening behaviour.

[1] Stricker M, Gagel J, Schmitt S, Schulz K, Weygand D, Gumbsch P., Meccanica 2015

[2] Zhang X, Aifantis KE, Senger J, Weygand D, Zaiser M., J Mater Res 2014;29:2116

[3] Senger J, Weygand D, Kraft O, Gumbsch P., Model Simul Mater Sci Eng 2011;19:74004

(E9 oral) **A crystal plasticity formulation for HCP metals informed by dislocation dynamics**

N Barton, M Messner, M Rhee and A Arsenlis

Lawrence Livermore National Laboratory, USA

We discuss a crystal plasticity model for hexagonal close packed (HCP) metals that has been developed to better capture detailed results of dislocation dynamics simulations. The dislocation dynamics simulations provide information about both dislocation density and flow stress evolution. In order to track dislocation density evolution appropriately, it is found that it is important to account for the effects of dislocation reactions among populations of gliding dislocations. A conventional hardening matrix is used to capture flow response interactions among dislocation populations, and it is found that the form of this hardening matrix is influenced by the proper accounting for the reactions among gliding dislocation populations. The new model is better able to reproduce the results of discrete dislocation simulations, in particular the development of dislocation density on inactive slip systems, while still capturing the expected latent hardening effect on the crystal-scale stress-strain response. It is possible that judiciously chosen experiments could verify the observed dislocation junction formation mechanisms and their influence on the response of the material. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-681127).

(E9 oral) **Dislocation multiplication by glissile junction formation in discrete dislocation dynamics and crystal plasticity**

M Stricker[1], F Roters[2] and D Weygand[1]

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The prediction of mechanical material properties relies on accurate modelling of the underlying microstructure processes. In continuum crystal plasticity models, the correct averaging procedures and rate formulations for the evolution of the dislocation densities and interactions are therefore necessary. Discrete Dislocation Dynamics simulations have shown that the dislocation multiplication due to the glissile junction contributes significantly to both dislocation density and plastic slip [1]. These findings are included into a continuum framework [2] through a rate formulation for the formation of glissile junctions. While macroscopic material parameters like yield stress do not differ significantly if the glissile junction formation is switched off, the resulting microstructure topology after straining is different. The role of the new multiplication mechanism in the extended crystal plasticity model is shown with heterogeneous density distributions (e.g. pre-straining, small samples): Glide systems, which otherwise would not be active are populated and contribute to the macroscopic deformation.

By enhancing continuum models with the microstructure-informed evolution equations for dislocation densities, including topology changes, a realistic state of the averaged microstructual variables is achieved.

[1] M. Stricker, D. Weygand, Dislocation multiplication mechanisms – Glissile junctions and their role on the plastic deformation at the microscale, Acta Mater., 99, 130 (2015)

[2] F. Roters, P. Eisenlohr, C. Kords, D.D. Tjahjanto, M. Diehl and D. Raabe, DAMASK: the Düsseldorf Advanced MAterial Simulation Kit for studying crystal plasticity using an FE based or a spectral numerical solver, Procedia IUTAM, 3, 3 (2012)

(E9 oral) **Predictions on the influence of microstructure variations on property scatter in additive manufacturing**

C Panwisawas, Y Sovani, M J Anderson, R P Turner, J W Brooks and H C Basoalto

University of Birmingham, UK

A multiscale multiphysics approach to modelling of additive manufacturing for aerospace materials is presented. Microstructural variability induced by the liquid/solid interactions resulting from selective laser melting (SLM) are known to influence the mechanical behaviour of a component producing scatter in material properties that can be location specific. The aim of this work is to develop a microstructure-based approach for the determination of optimised SLM parameters. The integrated computational materials engineering framework presented is based on an understanding of the causal-and-effect relationships between alloy microstructure, process route and component integrity. The physics-based models developed are applied to SLM of both titanium alloys and nickel-based superalloys. Processing-induced porosity resulting from a single pass laser scan is predicted using a computational fluid dynamics calculation which considers the representative powder-bed particle distribution derived from measurements. Thereafter, predicted as-fabricated grain microstructure – both grain morphology and texture – is obtained from a cellular automaton finite element calculation. A gamma double prime precipitation model is used to predict particle dispersion in the nickel-based superalloy 718. The micro-scale predictions for porosity, grain size and particle precipitation are fully linked with a macro-scale finite element calculation to predict residual stress and distortion using a microstructure sensitive dislocation-density based crystal plasticity model. It is demonstrated that the model predictions for the SLM process are sensitive to the microstructure details and can have a significant impact upon the overall integrity. The proposed framework provides a multiscale materials approach to simulate the additive manufacturing process.

(E9 oral) **Rafting of single crystal Ni-based superalloys: results from a coupled phase-field and continuum dislocation dynamics model including climb**

R Wu and S Sandfeld

University of Erlangen-Nuremberg, Germany

Controlling the directional coarsening (rafting) in Ni-based superalloys during creep loading is a key for extending the life time of many technologically relevant components as e.g. turbine blades. Up to now, predicting the interplay between precipitate microstructure evolution and resulting creep properties during rafting are still challenging, since a number of complex mechanisms on different time scales are involved.
We present results from a meso-scale continuum model which is able to reach time scales that are not accessible to molecular or discrete dislocation dynamics simulations. In our combined glide-climb continuum dislocation dynamics (CDD) model the motion of edge dislocations is represented based on dislocation density descriptions. The γ/γ' evolution is governed by a phase-field model (PFM). The coupling between CDD and PFM is mainly reflected through two aspects: the resolved stress from the γ/γ' misfit influences the dislocation motion, while dislocation eigenstrains contribute to the free energy governing the γ/γ' evolution. We analyse in detail the influence of climb, misfit and precipitate geometry on the resulting deformation behaviour. We show that our coupled CDD-PFM model can well - and in agreement with experimental data - predict the evolution of the γ/γ' morphology, the dislocation structure, as well as the resulting creep curves.

(E10 invited) **Computational modelling of dislocations microstructure in deformed crystals and comparison with 3D X-ray microscopy**

A El-Azab[1], S Xia[1] and B Larson[2]

[1]Purdue University, USA, [2]Oak Ridge National Laboratory, USA

We present a continuum dislocation dynamics model for mesoscale plasticity that predicts the formation of dislocation cell structure under monotonic loading of copper, in conjunction with the famous similitude law for the dependence of cell size on stress, and the dislocation vein structure under cyclic loading. This model features dislocation transport equations coupled with crystal mechanics, plus a closure problem consisting of finding the spatial and temporal correlations of the dislocation system. Our approach has been used to obtain a full solution of the deformation problem, which includes the dislocation pattern, deformation pattern and distorted shape, internal elastic fields, and stress-strain response and the dependence of all of the above on the loading direction. The results reveal the critical role of cross slip in cell structure formation under monotonic loading, as well as the relatively lower impact of cross slip when cyclic loading is applied. We give a short review of the model and sample key results along with a comparison of results with 3D X-ray microscopy data.

(E10 oral) **Multiple-slip continuum dislocation dynamics simulation of dislocation evolution in micro-beams**

A Ebrahimi and T Hochrainer

Universität Bremen, Germany

Plastic deformation of crystallite materials is driven by the motion and interaction of dislocations. Continuum Dislocation Dynamics (CDD) introduces flux-type evolution equations not only for geometrically necessary dislocations but also for the total dislocation density. CDD has been shown to predict plastic shear and dislocation densities in close accordance with Discrete Dislocation Dynamics (DDD) simulations while keeping the computation costs reasonably low. In previous work we presented simulations of the bending of a micro-beam composed of an fcc single crystal with only one activated slip plane. However, in highly symmetric crystal orientation relative to the bending load, plastic shear occurs simultaneously on multiple slip planes.

In the current work we present an implementation of CDD as a crystal-plasticity material law in form of a User-Material-Subroutine (UMAT) for the commercial finite-element solver ABAQUS. With this code we preform bending simulations of micro-beams with multiple activated slip systems for different beam dimensions and aspect ratios. We implement CDD as a crystal-plasticity material law and provide a User-Material-Subroutine (UMAT) for the commercial finite-element solver ABAQUS. The mechanical responses and the dislocation microstructure are compared with DDD simulations and available experimental results of bending of micro-beams. We show that CDD captures size effects, the evolution of the dislocation structure and the distribution of plastic shear in close accordance with DDD simulations.

(E10 oral) **Impact of atomic scale segregation effects on microstructural evolution in binary magnesium-rare earth alloys**

I Basu, K G Pradeep, C Mießen, L Barrales-Mora and T Al-Samman

RWTH Aachen University, Germany

This study develops non-Schmid constitutive models at two length scales, and bridges these length scales in a multi-scale framework. The constitutive models address thermo-mechanical behaviour of the Nickel-based superalloys for a large temperature range of 300K to 1300K, and include orientation dependencies of the constitutive models result in asymmetry in tension and compression for almost all orientations on the standard unit triangle. However simulations show different trends for the stronger direction (tension and compression) in terms of yield stress and hardening. For orientations close to [001] tension is the stronger direction while the behaviour is reversed by approaching to orientations close to [011] and the asymmetry disappears by approaching to [111] orientations. For the first length scale examined, the sub-grain scale, a size-dependent, dislocation density-based FEM model of the representative volume element (RVE) with explicit depiction of the morphology is developed as a building block for homogenization. For the next scale, an activation energy-based crystal plasticity (AE-CP) model is developed for single crystal *Ni*-based superalloys that can be implemented in simulations of polycrystalline aggregates. The homogenized AE-CP model develops functional forms of constitutive parameters in terms of characteristics of the sub-grain microstructural morphology. The homogenized parameters are expressed as functions of shape, volume fraction and channel-width in the sub-grain microstructure. The homogenized model has the advantage of significantly expediting crystal plasticity FE simulations due to parameterized representation of the morphology, while retaining accuracy with respect to the explicit representation.

(E10 oral) **Multiscale modelling of a-boron and boron carbide**

P Pokatashkin[1], P Korotaev[2] and A Yanilkin[2]

[1]All-Russia Research Institute of Automatics, Russia, [2]Dukhov Research Institute of Automatics, Russia

Boron carbide has a unique mixture of properties: low density, superhardness, high thermal stability, etc. It is used in personal armor, cutting tools, abrasives etc. Still, a good microscopic model of deformation is absent, as behavior of boron carbide under compression differs from other ceramics. We could mention the formation of narrow amorphous zones (1-3 nm thin) after ballistic impact, nanoindentation etc. Key research questions are: how the properties of damaged boron carbide differ from a pristine one and what are the critical conditions of appearing of these zones.

Though *ab initio* modelling is very accurate, its computational complexity makes nearly impossible studying of large systems, which is crucial for crystal defects. Therefore, in order to use classical molecular dynamics, interatomic potentials for α-boron and boron carbide were constructed. It is much easier to develop a potential for one element than for a binary system. That is why we also study α-boron as its structure and properties are quite similar to boron carbide.

Grain sliding across thin amorphous zones is studied by means of classical molecular dynamics. Shear strength dependency of damaged a-boron and boron carbide on pressure, temperature, strain rate is obtained. Evolution of amorphous zones is also studied. The results obtained could be used to define input parameters of hydrostatic models more accurate.

(E10 oral) **Microstructure formation during alloying reactions in nanofoils**

V Turlo, O Politano and F Baras

Universite de Bourgogne, France

The self-sustained propagating reactions occurring in Ni-Al nanometric metallic multilayers(N2Ms) was studied by means of molecular dynamics (MD) and macroscopic modelling. N2Ms are made of hundreds of thin layers of metals deposited alternately. They are highly reactive and can be locally ignited leading to the formation of a propagation front crossing the whole sample without any further supply of heat. We studied the relation between microstructure and front propagation.

Large scale microscopic MD simulations were performed to include mass and heat transfer. Various physical mechanisms were observed and described, such as dissolution and intermixing, nucleation of intermetallic grains, grain coarsening and recrystallization of the final products. Phenomenological models of these transformations were proposed to analyse atomistic simulations and assess parameters with a good agreement with available experimental data. This study allowed to determine the processing parameters which control the microstructure.

(E11 invited) **Multiscale modelling of microstructure evolution in polycrystalline materials: physical and numerical challenges**

R Lebensohn

Los Alamos National Laboratory, USA

Emerging materials characterization methods and micromechanical formulations are enabling the discovery of complex relationships between processing, microstructure and properties in polycrystalline materials, as well as the implementation of numerically-tractable multiscale approaches to represent these relationships at the scale of engineering components.

Full-field formulations, requiring the consideration of a huge amount of degrees of freedom, allow both the rationalization of these relationships directly from data generated by 3-D characterization techniques, as well as the generation of reference solutions for validation of more efficient microstructure-aware models amenable to be implemented in multiscale formulations.

In this talk we report on recent advances in Fast Fourier Transform-based models, which can use direct input from voxelized microstructural images to predict the micromechanical and effective response of polycrystalline materials, and their use for validation of novel homogenization-based and semi-analytical models to represent processing-microstructure-property relationships in engineering applications.

(E11 oral) **High-temperature plasticity of nanograined boron carbide polycrystals**

D Gomez Garcia, B M Moshtaghioun and A Dominguez-Rodriguez

University of Seville, Spain

Boron carbide ceramics are among the most promising materials as a result of its outstanding room temperature mechanical properties. This is the third hardest material in Nature after diamond and cubic boron nitride.

Despite its potential applications, the fabrication of this material is a challenging task due to the low values of the self-diffusion coefficients. Quite recently this goal has been achieved by means of spark plasma sintering.

This presentation outlines the high-temperature creep response of fully-dense nanograined boron carbide polycrystals. Contrary to the well-established ideas, the equation of state of creep does not follow the current power law derived from recovery creep. An analytical model is proposed to explain the main experimental features measured in creep tests. The model will be assessed by transmission electron microscopy observations. The consequence for creep hardening will be addressed.

(E11 oral) **Heterogeneous deformation in nickel-based superalloys**

H Basoalto[1], G Yearwood[1], J Rangel[1], A Mello[2], M Sangid[2] and J Brooks[1]

[1]University of Birmingham, UK, [2]Purdue University, USA

The presence of the intermetallic g¢ phase in nickel-based superalloys has a strong effect on the mechanical response of these alloys and is responsible for the heterogeneous slip observed in these materials. Hence, their development has been primarily driven by tailoring chemistry and processing routes to increase volume fraction and multi-modal particle size distributions to achieve the required properties. A constitutive description of the high temperature plastic flow in precipitate strengthened alloys will be presented, which is based on a diffusion-reaction equation for the mobile dislocation density that accounts for the multimodal particle dispersion. The constitutive relations are implemented within a finite element crystal plasticity formulation to determine the macro-scale behaviour. The proposed multi-scale model accounts for a number of micromechanisms that include dislocation climb around particles and shear of the γ' precipitates. Predictions of the heterogeneous deformation are presented, which relate the location of deformation to the particle distribution resulting from different heat treatments. In-situ strain maps have been measured for the nickel-based superalloy RR1000 exposed to two different heat treatments producing fine and coarse particle dispersions. The strain maps obtained under uniaxial loading conditions at room temperature clearly show differences in the distribution of strains and this heterogeneity is show to be consistent with the model predictions.

(E11 oral) **A spectral method to solve multi-physics coupled elasto-viscoplastic boundary value problems**

P Shanthraj, S Zhang, L Sharma, F Roters and D Raabe

Max Planck Institut für Eisenforschung, Germany

In the last decade, the spectral method has emerged as an efficient alternative to the widely used finite element method (FEM) for the prediction of the underlying micromechanical response of structural materials, and has more recently been extended to treat finite deformations and general constitutive laws. While application of the spectral method to purely mechanical boundary value problems has received considerable attention, its application to possibly time-dependent and interacting field equations representing coupled multi-physics systems has been relatively unexplored.

To address this shortcoming, the objective of this thesis is to develop a spectral solution scheme for the time-dependent reaction-diffusion equation, which is representative of several field equations of interest such as thermal conduction, non-local damage and more general phase-field equations. The solution scheme will be based on using the analytic Green's function for the homogeneous time-dependent diffusion equation, while treating the heterogeneous and reaction terms iteratively, in an analogous manner to the treatment of the polarization field mechanical spectral solver. The solution scheme will be implemented in the Düsseldorf Advanced Material Simulation Kit (DAMASK) and solved self-consistently with existing solvers and constitutive laws for the mechanical boundary value problem. The numerical strengths and weaknesses of the solution scheme will be assessed in the context of a polycrystalline material undergoing coupled thermo-damage-mechanical deformation using available crystal plasticity, damage and thermal constitutive laws.

(P1.22) **Ultrasonic techniques to detect dislocation proliferation**

V Salinas, N Mujica, R Espinoza and F Lund

Universidad de Chile, Chile

Ultrasound (US) has been in use for decades as a nondestructive testing tool [1]. The detection of cracks and flaws in solid materials in service is a major field of application [2]. One mode of failure is ductile failure or plastic yield, which is governed by the proliferation of dislocations [3]. Can US be used as a nondestructive testing tool for the plastic behavior of materials in the same way that it is used to test for brittle fracture? We here report results of local insitu measurements of the speed of shear waves, vT, in aluminum under standard testing conditions (traction test), as a function of externally applied stress. There is a clear decrease in vT at the yield stress, consistent with a proliferation of dislocations. These measurements provide a quantitative, continuous relation between dislocation density and externally applied stress, and paves the way for the development of US as a diagnostic tool of dislocation density for metallic pieces in service where other methods, such as X-ray diffraction (XRD) and transmission electron microscopy (TEM) are not available because of their destructive nature on preparation of samples.

We acknowledge the support of Fondecyt Grant 1130382 and 3160164.

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(P1.30) **Micro-mechanical analysis of oxide dispersion strengthened ferritic steel tubes transformed by cold pilgering mill**

E Vakhitova[1], D Sornin[1] and M François[2]

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Ferritic oxide dispersion strengthened (ODS) steels can be applied as a material for advanced type reactors. Metallurgical investigations of ODS steel tubes produced by hot extrusion of powder material and followed by cold pilger rolling are considered in the present work. Determination of the process parameters influence on the microstructure evolution at the industrial scale is carried out. Experimental and numerical research is required in order to understand the material behaviour after several steps of treatment, namely hot extrusion of powder material, cold pilgering and heat treatment. A microstructure analysis is performed considering 9Cr and 14Cr-ODS ferritic steels. The shape, size and orientation of the grains were obtained by Scanning Electron Microscopy (SEM), Electron Backscattering Diffraction (EBSD) and X-ray Diffraction analyses (XRD). Macroscopic residual stresses and intergranular stresses are followed by XRD at each step of the thermo-mechanical treatment.

The deformation process of ODS tubes can be simulated using different constitutive models for predicting the material behaviour. A polycrystalline plasticity code is used for numerical modelling of the strongly anisotropic microstructure of ODS tubes. It allows to follow the texture evolution with plastic deformation and predict the mechanical response of the material (yield stress and work-hardening). It also enables to estimate the intergranular stress heterogeneity arising from local strain incompatibilities. The results are then compared with the experimental observations.

(P1.31) **Novel application of potts model for grain growth during welding using SPPARKS**

J Mitchell and V Tikare

Sandia National Laboraties, USA

The model presented in this paper simulates grain growth during welding in the vicinity of the weld. The model simulates the effects of velocity and shape of molten weld pool, and geometry and shape of heat affected zone (HAZ) on the resulting grain structure by melting the region within the molten pool and varying grain boundary mobility *M* based upon geometric proximity (alias for local temperature) to the weld pool. The model is implemented in the SPPARKS framework for kinetic Potts Monte Carlo simulations and qualitatively predicts trends in spatial and temporal microstructures relevant to real weld processes. Spatial/geometric statistics, such as grain size and number of grains through thickness of weld, are calculated and presented.

(P2.18) **Enhanced degradation of Zirconia ceramics upon water incorporation: a DFT investigation**

A Gebresilassie[1], T Albaret[1], L Gremillard[2], J Chevalier[2] and A Gebresilassie[1]

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During the 1990's Yttriated zirconia ceramics, i.e. ZrO2 doped with 3% to 6% Y2O3, became a prototypical material for several surgery implants. The reason is the high fracture toughness of this ceramic which is partly due to a fascinating Phase-Transformation-Toughening mechanism [1] involving a stress driven transformation from a tetragonal phase (T) towards a more stable monoclinic phase (M). However, in presence of water, the same phase transformation can spontaneously occur, leading to the global failure of the material [2].

In this work we aim at understanding the elementary mechanisms responsible for the water induced degradation of this material by conducting Density Functional Theory calculations using several functionals (LDA-GGA) on pure and Yttriated zirconia bulk systems to which we incorporated water molecules.

In close correspondence with the experimental phase diagram, we will first discuss the stability of the pure and defected systems as a function of the iono-covalent character of the Zr-O bonds. Then we will present the calculations on the systems containing water molecules which provide some insight on the water induced degradation mechanism. Our main results indicate that the mechanism is energetically driven, while some specific structural effects due to the dissociated water in the material can be evidenced from solid-state NEB calculations[3] that mimic the T to M transformation.

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(P2.19) **Effects of fcc/fcc grain boundaries on the formation of bcc phase in pure iron by molecular dynamics simulation**

X Ou, J Sietsma and M J Santofimia

Delft University of Technology, Netherlands

Molecular dynamics simulations were used to study the effects of three different fcc/fcc grain boundaries, with different misorientations, on the nucleation and growth of bcc phase in pure iron. The studied fcc/fcc grain boundaries were: one low-angle grain boundary (LAGB), one high-angle grain boundary (HAGB) and one coherent twinning boundary. The LAGB and the HAGB were constructed by rotating part of a single fcc crystal by about 5° and 45° around the $[0\ 1\ 0]_{fcc}$ direction, respectively. The LAGB is semi-coherent with periodic dislocations, while the HAGB is incoherent. Heterogeneous nucleation of bcc phase was found to take place at both the LAGB and the HAGB, whereas homogeneous nucleation was not observed. The nuclei forming at the coherent part of the LAGB shows a Kurdjumov-Sachs (KS) orientation relationship with both parent fcc crystals. The nuclei forming at the incoherent part of the LAGB or at the HAGB has a special orientation relationship with one of the parent fcc crystals, either in the Pitsch Orientation or the KS orientation. No phase transformation was observed for the coherent twinning boundary after a simulation time of 100 ps. It was estimated that the newly formed bcc/fcc interfaces propagated into the original fcc phase at an velocity on the order of 1000 m/s, which exhibits a martensitic nature.

Symposium F

(F1 invited) **Enhanced free energy based structure prediction in materials science**

M Tuckerman, E Schneider, L Vogt, M Chen and T-Q Yu

New York University, USA

Theory and computation, in synergy with experiment, are playing an increasingly important role in the design and characterization of new materials. In this talk, I will describe the efforts we are making in my group to develop new computational methodologies that address specific challenges in materials modeling. In particular, I will describe our recent development of enhanced free energy based methodologies for predicting structure and polymorphism in molecular crystals and for determining conformational equilibria of oligopeptides. The strategies we are pursuing include heterogeneous multiscale modeling techniques, which allow "landmark" locations (minima and saddles) on a high-dimensional free energy surface to be mapped out, and temperature-accelerated methods, which allow relative free energies of the landmarks to be generated efficiently and reliably. Results from applications to small, bound peptides and various atomic and molecular crystals, including one of the targets from the recent CCDC sixth blind structure prediction test, and co-crystals will be presented. I will also discuss the application of our computational protocol in the study of first-order phase transitions. Finally, future directions and challenges will be highlighted.

(F1 oral) **Cross-entropy minimization and importance sampling of rare events**

C Hartmann and W Zhang

Freie Universität Berlin, Germany

Cross-entropy (CE) minimization is a versatile Monte Carlo method for combinatorial optimization and sampling of rare events, which goes back to work by Reuven Rubinstein and co-workers. I will report on recent algorithmic extensions of the CE method to diffusions that can be used to design efficient importance sampling strategies for computing the rare events statistics of equilibrated systems. The approach is based on a Legendre-type duality between path functionals of diffusion processes associated with certain sampling and control problems that can be reformulated in terms of CE minimization. The method will be illustrated with several numerical examples and discussed along with algorithmic issues and possible extensions of the method to high-dimensional multiscale systems. Related approaches based on large deviations asymptotics and the geometric Miminum Action Method (gMAM) will be discussed during the talk.

(F1 oral) **Comparison of minimum action and steepest descent paths in gradient systems**

G D Leines and J Rogal

Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Germany

On high dimensional and complex potential energy landscapes, the identification of the most likely mechanism of a rare reactive transition is a large challenge. The minimum energy path (MEP) is a widely used reaction path (RP) model defined by the steepest descent (SD) trajectories from a saddle to the minima. Although the MEP is very often associated with the most likely path, its local approximation of using only the potential gradient to determine the RP might not always capture other possibilities of curvature and global characteristics of complex PESs. In particular, on PESs with bifurcation points and multiple minima and saddles, several MEPs can connect two predetermined minima and the identified trajectory can largely differ from the path of maximum likelihood.

Here we present a comparison of the SD-based definition of the MEP to the path integral formulation of a trajectory that minimizes an action functional for Brownian dynamics. We show that the minimum action path additionally takes into account the scalar work, which provides a measure of the likelihood of the identified mechanisms in gradient systems. In particular, the scalar work can be used to distinguish between various steepest descent paths in multiple state transitions, and serve as a RP model near ridges, when bifurcations occur.

We illustrate that in systems with non-trivial energy landscapes the evaluation of the action can provide valuable information for the analysis and description of the most likely path, and alleviate some of the limitations of the MEP to model complex transitions.

(F1 oral) **Nested sampling of reaction paths**

G Csanyi

University of Cambridge, UK

I will demonstrate the application of Nested Sampling, a thermodynamically accurate and efficient global sampling strategy, to the problem of reaction path sampling. Nested Sampling is a top-down scheme, which starts with the high-entropy-low-likelihood region of configuration space and systematically works its way down to the low-entropy-high-likelihood modes of the desired probability distribution. It is especially efficient for systems with phase transitions, where the entropy changes rapidly for small changes in likelihood.

(F2 invited) **Energy landscape and pathways of point defects in body-centered-cubic metals**

M-C Marinica[1], W Unntoc[1], M Athènes[1], G Stoltz[2] and T Lelièvre[2]

[1]CEA, Université Paris-Saclay, France, [2]Université Paris-Est, France

Progress in future energy systems depends critically on our ability to design new materials with adequate properties under extreme conditions. Properties of small defect clusters such as vacancies or interstitials underpin any multi-scale model predicting the evolution of materials under extreme conditions [1]. This study aims at improving our understanding of the free energy landscape of point defects in body-centered-cubic metals up to the melting temperature by resorting to atomistic simulations based on electronic structure calculations. The phase space is sampled using adaptive molecular dynamics methods [2-4] and ab initio atomic forces. Moreover, taking advantage of versatility of adaptive free energy methods we combine the *ab-intio* force field with interatomic machine learning based interactions. The present approach merging ab initio – free energy – machine learning methods, can provide quantities such as formation free energies or diffusion transition rates as key input parameter for any subsequent multi-scale simulation. In the case of tungsten, candidate material for first wall and divertor components of future fusion reactors, our results will be directly compared with the experiment.

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(F2 oral) **Metadynamics simulations of phase transitions in crystalline and amorphous ice**

S Pipolo, G Ferlat, M Salanne, M Saitta and F Pietrucci

Université Pierre et Marie Curie, France

Using Molecular Dynamics (MD) to simulate phase transitions is a challenging task due to the big gap between the physical timescales the ones accessible to simulations. Among the different MD accelerating techniques, metadynamics [1] provides a powerful tool to overcome such limitation and to reconstruct the free-energy landscape. The definition of a suitable collective variable tracking the transition mechanism is the key problem and it is strongly process-dependent. Since, in general, phase transitions encompass both short-range chemical changes and long-range collective processes, finding good coordinates is highly non-trivial.
We propose a definition that combines the Path Collective Variable (Path-CV) [2] and the Permutation Invariant Vector (PIV) [3]. This allows to trace a continuous path between the two phases in a two-dimensional space and accounts for the topological complexity of the structures through the PIV metrics. We apply such methodology to different phase transitions between crystalline and amorphous ice phases, exploring the mechanisms and energetics of the processes at different thermodynamics conditions (pressure and temperature) by computing free-energy barriers and transition paths [4].

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(F2 oral) **Nucleation and interfacial adsorption in ternary systems**

T Philippe

CNRS, Ecole Polytechnique, France

Nucleation is studied in incompressible ternary fluids by examining the overall landscape of the energy surface. Minimum free energy paths for nucleation (MFEPs) of a single nucleus in an infinite matrix are computed with the string method in the framework of the continuum theory of nucleation for the regular solution. Properties of the critical nucleus are compared with the predictions of the classical nucleation theory. MFEPs are found to exhibit complex nucleation pathways with non-monotonic variations of compositions in the interfacial region, specifically adsorption of a component. In the symmetric regular solution, the minority component is found to segregate at the interface during nucleation with a concomitant depletion of the nucleus core, resulting in unpredicted partition of the non-selective component. Despite increasing the gradient energy, such inhomogeneity in composition is shown to lower the nucleation barrier.

(F2 oral) **Estimating rates of thermally activated events by sampling and unbiasing dynamically activated paths**

M Athènes[1], P Terrier[2] and M-C Marinica[1]

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Transition path sampling is a rare-event method that estimates state-to-state time-correlation functions in many-body systems from samples of short trajectories and then extracts rate constants from the time derivatives of the estimated correlation functions. In this framework, it is proposed to bias the importance function so as to favor trajectories exploring negatively curved portions of the potential energy surface. Because metastable basins are separated from each other by mechanically unstable regions, the biasing approach favors the sampling of activated trajectories and increases the occurrence of the rare reactive trajectories of interest, those corresponding to transitions between locally stable states. Estimating the time-correlation functions involves unbiasing the sample of simulated trajectories which is done using a novel procedure based on Bayes formula and known as conditioning in probability theory. To assess the performance of our procedure, we compute the time-correlation function associated with the migration of a vacancy in α-iron. The derivative of the estimated time-correlation function yields a migration rate in agreement with the one given by transition state theory. Unlike original transition path-sampling, our approach requires neither computing the reversible work to confine the trajectory endpoints to a reactive state nor postprocessing the harvested correlation functions.

(F2 oral) **Scale transition using dislocation dynamics and the nudged elastic band method**

L Capolungo[1], C Sobie[2], D McDowell[2] and E Martinez[1]

[1]Los Alamos National Laboratory, USA, [2]Georgia Institute of Technology, USA

Dislocation dynamics simulations have been used extensively to predict hardening caused by dislocation-obstacle interactions, including irradiation defect hardening in the athermal case. Incorporating the role of thermal energy on these interactions is possible with a framework provided by transition state theory. Unit dislocation-defect reaction processes are within reach of atomistic calculations, but the scale transition of information at the nano-scale to representative volumes is unclear. In this work, the NEB method is generalized to coarse-grain continuum representations of evolving microstructure states beyond the discrete particle descriptions of first principles and atomistics. A novel method is proposed using continuum discrete dislocation dynamics to calculate activation energies for dislocation bypass of obstacles using NEB. The significant increase in computational speed compared to atomistic simulations enables the calculation of activation energies for a 1/2 [111] (1-10) glide dislocation bypassing a [001] self-interstitial atom loop of size in the range of 4-10 nm in bcc iron for a range of applied stresses and interaction geometries. Moving beyond unit dislocation-defect reactions to a representative environment containing a large number of defects requires coarse-graining the activation energy barriers of a population of obstacles into an effective energy barrier that accurately represents the large scale collective process. The work presented here investigates the relationship between unit dislocation-defect bypass processes and the distribution of activation energy barriers calculated for ensemble bypass processes. A significant difference between these cases is observed, which is attributed to the inherent cooperative nature of dislocation bypass processes.

(F3 invited) **Hierarchical dynamics of biomolecular processes**

G Stock

University of Freiburg, Germany

Biomolecules exhibit structural dynamics on a number of timescales, say, from 10^{-12} to 10^{1} seconds. Despite this substantial separation of timescales, fast and slow degrees of freedom appear to be coupled in a nonlinear manner, e.g, there is theoretical and experimental evidence that fast structural fluctuations are required for slow functional motion to happen. Adopting Aib peptide as a simple model system, we perform extensive molecular dynamics simulations to discover a hierarchy of (at least) three tiers of the molecule's free energy landscape [1]. Providing a simple mechanism of hierarchical dynamics, picosecond hydrogen bond dynamics is found to be a prerequisite for the nanosecond local conformational transitions, which in turn are a prerequisite for the microsecond global conformational rearrangement of the peptide. As a consequence of the hierarchical coupling, the various processes exhibit a similar temperature behavior which may be interpreted as a dynamic transition.

Using principal component analysis techniques to define a five-dimensional essential space, the hierarchical energy landscape and conformational dynamics of the system is modeled by a data driven Langevin equation [2]. As the multidimensional Langevin fields describing deterministic drift and stochastic driving are estimated locally, the method can be used in enhanced sampling methods such as the construction of the overall energy landscape of a system from short trajectories.

[1] S. Buchenberg, N. Schaudinnus and G. Stock, "Hierarchical biomolecular dynamics: Picosecond hydrogen bonding regulates microsecond conformational transitions", J. Comp. Theo. Chem. 11, 1330 (2015)

[2] N. Schaudinnus and B. Bastian and R. Hegger and G. Stock", "Multidimensional Langevin modeling of nonoverdamped dynamics", Phys. Rev. Letters 115, 050602 (2015)

(F3 oral) **Long-time atomistic simulations with Parallel Trajectory Splicing**

D Perez and A Voter

Los Alamos National Laboratory, USA

Molecular Dynamics (MD) is a workhorse of computational materials science. Indeed, MD can in principle be used to obtain any thermodynamic or kinetic quantity, without introducing approximation or assumptions beyond the adequacy of the interaction potential. This enviable quality however comes at a steep computational price, hence limiting the system sizes and simulation times that can be achieved in practice. While the size limitation can be efficiently addressed with massively parallel implementations of MD based on spatial decomposition strategies, the same approach usually cannot extend the timescales much beyond microseconds. In this talk, we discuss a novel approach - Parallel Trajectory Splicing (ParSplice) - that aims at addressing the timescale limitation of MD for systems that evolve through rare state-to-state transitions. As with the Parallel Replica Dynamics method, the problem is instead parallelized in the time domain. The key innovation of ParSplice lies in the use of speculation on the future evolution of the dynamical trajectory. This exposes additional parallelism by allowing work to simultaneously proceed in many states. Predictions are carried out through a concurrent stochastic simulation parameterized on the fly. We review the formal underpinnings of the method and demonstrate that it can provide arbitrarily accurate results while providing significant improvement in computational efficiency compared to its predecessors. We then illustrate the usefulness of ParSplice by presenting different examples of materials simulations where access to long timescales was essential to access the physical regime of interest.

(F3 oral) **Error estimates for transport coefficients in molecular dynamics**

G Stoltz

Ecole des Ponts, France

I present error estimates for transport coefficients, which can be obtained either by the linear response of appropriately perturbed stochastic dynamics, or, equivalently, through the time integration of correlation functions. I consider two issues: the reduction of the bias arising from the numerical integration of continuous dynamics (typically, Langevin dynamics integrated with splitting schemes), and the reduction of the variance through appropriate variance reduction techniques for nonequilibrium systems.

(C4+F4 invited) **Continuum modeling of heteroepitaxial growth in semiconductors**

F Montalenti[1], F Rovaris[1], R Bergamaschini[1], M Salvalaglio[1], M Albani[1], L Miglio[1], R Backofen[2] and A Voigt[2]

[1]Università di Milano-Bicocca, Italy, [2]Universitat Dresden, Germany

Integration of different materials, such as GaAs or Ge, on Si via heteroepitaxy is nowadays a key step involved in the fabrication of a multitude of devices. However, full control over the different, sometimes competing phenomena taking place during deposition [1] has yet to be reached. Simulations can be precious in limiting the growth-parameter space to be sampled in actual experiments when searching for the desired system quality and morphology.

In this work we present a continuum approach able to tackle heteroepitaxy while matching typical experimental sizes and time scales. A convenient and general description of surface-energy anisotropy is introduced [2] and several illustrative applications to semiconductors are described, exploiting both Phase-Field and sharp-interface approaches. Successful comparison with experiments is demonstrated [3].

We also discuss how to simultaneously tackle elastic and plastic relaxation. In particular, we show how the stress field associated with an assigned distribution of misfit dislocations can be computed on the fly, its contribution to the surface chemical potential deeply influencing the growth mode and/or the morphology of the growing front.

[1] F. Montalenti et al, Comptes Rendus Physique **14**, 542-552 (2013)
[2] M. Salvalaglio et al, Cryst. Growth Des. **15**, 2787 (2015)
[3] M. Salvalaglio et al, ACS Appl. Mater. & Interf. **7**, 19219 (2015)

(C4+F4 oral) **Elementary mechanisms of shear-coupled grain boundary migration**

N Combe[1], A Rajabzadeh[1], F Mompiou[2] and M Legros[2]

[1]CEMES, CNRS UP 8011 and Univ Paul Sabatier, France, [2] Universite de Toulouse, France

Nanocrystalline materials (grains sizes Investigating the minimum energy path of the Σ13 (320) and Σ17(410) GB migration in a copper bicrystal, the GB migration is shown to occur through the nucleation and motion of GB steps identified as disconnections. Energy barriers for the GB and disconnection migrations are evaluated [1,2].

For the Σ17(410) GB, both and GB migration modes are compared. The atomic mechanisms of both modes qualitatively differ: while the mode presents no metastable state, the mode shows multiple metastable states, some of them evidencing some kinks along the disconnection lines. Disconnection kinks nucleation and motion activation energies are evaluated. Besides, the activation energies of the mode are smaller than those of the one excepted for very high stresses.

[1] Rajabzadeh, A.; Mompiou, F.; Legros, M. and Combe, N. Phys. Rev. Lett., **110**, 265507 (2013)
[2] Combe N.; Mompiou, F.; Legros, M. Phys. Rev. B, accepted (2016)

(P1.32) **From glissile to sessile: influence of temperature on slip in perovskite materials**

P Hirel, P Carrez and P Cordier

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Compounds with the perovskite structure can exhibit very different mechanical properties. The archetypal perovskite material strontium titanate ($SrTiO_3$) presents a very atypical mechanical behavior, characterized by a double ductile-brittle-ductile transition. The plastic deformation at low temperature is accommodated by the motion of dislocations of <110> Burgers vector, however these dislocations suddenly loose their mobility around 1050 K, leading to brittle failure. The mechanisms responsible for the loss of this slip system are still unknown, and also raise the question of the existence of similar mechanisms in related compounds.

The effects of temperature on the core structure of <110> dislocations are investigated by means of atomic-scale simulations in two perovskites: $SrTiO_3$ because of its important technological applications, and $MgSiO_3$ because of its geophysical applications, as it is the most abundant mineral in the Earth's lower mantle. We demonstrate that in both phases, <110> dislocations transform from a glissile core spread in their slip plane, into a sessile, climb-dissociated core at high temperature. The results indicate that the mechanisms for this transformation may be general to all perovskites, with an activation energy that strongly depends on the chemical composition. This leads to a competition between this temperature-induced transformation and the stress-driven motion of dislocations. As a result the mechanisms for the deformation are extremely different depending on the conditions of deformation: at low temperature and high stress the glide of <110> dislocations dominates, while at high temperature and low stress <110> dislocations become sessile, and deformation has to occur by different mechanisms.

(P1.33) **Size-dependent potential energy landscapes of vacancy migration in ionic nano particles**

T Niiyama[1], T Okushima[2], K Ikeda[3] and Y Shimizu[3]

[1]Kanazawa University, Japan, [2]Chubu University, Japan, [3]Ritsumeikan University, Japan

Size dependence of vacancy diffusion in ionic nanoparticles is investigated by analysis of potential energy surfaces (PES) [1]. Elucidating the topological features of energy landscapes is indispensable for understanding the complicated dynamics of various materials, such as molecular, nanoparticles, crystals, etc. Vacancy diffusion in solids is one of the most simple dynamics that are captured by potential energy landscape perspectives. Rapid diffusion in nanoparticles that has been reported in experimentally and numerically might be understood by the perspectives.

Regarding PESs, we investigate size dependence of vacancy migration in ionic nanoparticles, namely potassium chloride clusters. The PES of the dynamics is visualized with a graph-based technique, so-called saddle-connectivity graph, by listing local minima and transition states for inter-site vacancy migration. From the results, we compute the vacancy migration energies and identify the most probable path for migration from the center of the cluster to a vertex. Common features of the PES in clusters of different sizes and dependence of PES on cluster size are discussed. In the inner core region of a cluster, the PES is uniform and migration energy is similar to that of a bulk crystal. In the outer region near the surface of a cluster the PES is rugged, and the migration energy is typically lower. The mean first-passage time for migration of a vacancy from the center to a vertex decreases with cluster size. These results are consistent with observations of higher diffusion rates in smaller clusters.

[1] T. Niiyama et al., Chem. Phys. Lett. (Submitted)

(P1.34) **Diffusion of vacancies in bcc metals and its dependence on temperature**

K Fidanyan and V Stegailov

Joint Institute for High Temperature of Russian Academy of Sciences, Russia

The generally accepted model for temperature dependence of diffusion of defects is the Arrhenius equation [1]. However, there is some evidence that the Arrhenius law is not accurate at high temperatures, when anharmonicity of atomic interactions cannot be neglected and makes a significant contribution to the formation and migration energy of defects [2]. There are recent discussions of temperature effects on the vacancy formation volume and consecutive effects on the mobility of vacancies [3].

This work present accurate description of the vibrational density of states required for calculation of defect migration rates in the Vineyard theory framework. We use EAM and MEAM interatomic potentials and apply the zero temperature lattice dynamics calculations and the velocity autocorrelation function calculations at finite temperatures to study vibrational density of states in bcc Mo and U lattices. The latter case is especially interesting since bcc U is unstable at low temperatures.

Direct molecular dynamics simulations of the motion of defects in bcc metals considered, reveals the deviation from the Arrhenius law. Temperature dependence of the migration energy is discussed, and the new techniques for evaluation of the pre-exponential factor are considered.

[1] Vineyard G, J. Phys. Chem. Solid 3 (1957) 121–127
[2] Glensk A, Grabowski B, Hickel T and Neugebauer J, Phys. Rev. X 4 (2014) 011018
[3] Valikova I and Nazarov A, In proc. conference Thermodynamics and Transport Kinetics of Nanostructured Materials (2009) 128–129

(P1.35) **Charge-variable interatomic potential for UO2 using a second moment tight-binding model**

D Mbongo[1], R Ducher[1], R Dubourg[1], R Tétot[2] and N Salles[3]

[1]IRSN, France, [2]Université Paris Sud, France, [3]LAAS-CNRS, France

The tight-binding variable-charge model SMTBQ is modified to better describe the iono-covalent character of U-O bond in the Uranium dioxide structure. In fact, the previous work on UO_2 based on the SMTBQ model [1-2] underestimates the electronic gap of this structure (0.6 eV), which is known experimentally to be around 2 eV. The difference comes mainly, from the fact that the splitting effect of 5f orbitals which is responsible of the gap opening, was not taken into account in the previous SMTBQ model. This work focus mainly on introducing the energy term, which we call ε_s, coming from the uranium 5f orbitals splitting due to the crystalline field of oxygen atoms. According to this new term, the covalent energy part can be written as:

$$Ecov =^{(1)} - 2 \times n_1 \times \varepsilon_s$$

As results, the structural properties and the cohesive energy calculated with this model are found in good agreement with the experimental data. The calculated charges on uranium and oxygen ions are respectively equal to 3.0 and -1.5.This charge-variable potential model is used, on one hand to investigate the stability of hyper-stoichiometric structure of UO_2 and on the other hand; to characterize the Mo-O interaction, in order to study the Mo behaviour in $UO_{2\pm x}$.

[1] G Sattonnay and R Tétot, *Phys.: Condens. Matter* **25** (2013) 125403
[2] Salles, O. Politano, E. Amzallag and R. Tetot, *Comput. Mater. Sci.* 111 (2016) 181-189

(P1.36) **Density functional theory calculations of vanadium carbides**

S E Restrepo[1] and A T Paxton[2]

[1]SKF, Sweden, [2]King's College London, UK

Stability

Vanadium carbide precipitates in steels can provide simultaneously improved hardness and hydrogen resistance. We have made first principles calculations of structural, mechanical and energetic properties of a variety of vanadium carbides, all of which are claimed from experiment to exist as precipitates in steels. Calculated values of the lattice parameters, formation enthalpy and stiffness tensor agree well with values found in the literature, when available.

These results are used to compare the carbides in terms of their energetic and mechanical stability, compressibility and ductility/brittleness. From these calculations, it is concluded that V6C5 with space group C2/m is the most stable among the considered variants.

Diffusion

Experimental observations using atom probe tomography [Takahashi2012] and small-angle neutron scattering [Malard2012] suggest that H can be trapped inside vanadium carbide precipitates in high strength steels. In contrast with those results, DFT calculations of the energetics and diffusion of H in V4C3 which is a commonly accepted composition for vanadium carbides suggest that the energy barriers that H would need to overcome in order to segregate into the precipitate are too high.

In the present study, the energy barriers for the diffusion of H within a V6C5 precipitate are obtained using DFT calculations and the minimum energy path method. It was found that despite the existence of "diffusion channels" that could allow H to travel within the precipitate, the energy barriers are still too high for the diffusion of H under operating conditions.

Symposium G

(G1 invited) **First-principles modelling of screw dislocation mobility in Zr and Ti**

E Clouet[1], N Chaari[1], D Rodney[2] and D Caillard[3]

[1]CEA Saclay / SRMP, France, [2]University Lyon 1, / ILM, France, [3]CNRS / CEMES, France

Titanium and zirconium have a close plastic behaviour arising from their hexagonal close-packed crystallography and from their similar electronic structure. In particular, plasticity in these two transition metals is controlled by screw dislocations gliding in the prism planes, with cross-slip in the first-order pyramidal planes or in the basal planes activated at high enough temperature and a strong hardening associated with O addition. We use ab initio calculations and NEB method to study core properties of the screw dislocations and their mobility in both metals. These calculations show that screw dislocations may adopt different cores that are dissociated either in a prism or in a pyramidal plane. The prismatic core easily glides in its habit plane, whereas the pyramidal core needs to overcome an important energy barrier to glide. The prismatic glissile core is the most stable in Zr, but the dislocation ground state in Ti corresponds to the pyramidal core. As a consequence, dislocation glide is easy and confined in the prismatic planes at low temperature in pure Zr, whereas a locking-unlocking mechanism operates in Ti where the locked periods correspond to a slow and limited glide in pyramidal planes and the unlocked periods to a rapid and extended glide in prismatic planes, in agreement with in situ TEM straining experiments. Finally, we study the interaction of an oxygen atom with these different configurations of the screw dislocation. Ab initio calculations evidence a strong repulsion with the oxygen repelling the stacking fault ribbon, thus inducing dislocation cross-slip.

(G1 oral) **Dislocation trajectory and Schmid law deviation in BCC metals**

L Dezerald[1], D Rodney[2], E Clouet[3], L Ventelon[3] and F Willaime[3]

[1]IJL, France, [2]ILM Lyon, France, [3]CEA Saclay, France

Plasticity in Body-Centered Cubic (BCC) metals arises from 1/2<111> screw dislocation glide. These dislocations are known to display strong core effects that are responsible for BCC metals' atypical properties at low temperatures such as a marked dependence of the elastic limit on crystal orientation, in clear violation of the Schmid law that applies to most other metals. Here, we propose a law based on DFT (Density Functional Theory) calculations of 1/2<111> screw dislocation properties to predict Schmid law deviation in BCC crystals. We show that at atomic scale, screw dislocations glide in {110} planes only on average. The path they follow is systematically shifted towards the twinning region. The amplitude of this deviation is metal dependent and can directly be linked to the dislocation Peierls potential, the two-dimensional energy landscape of the dislocation in the {111} plane. We consequently modified the Schmid law by projecting the applied stress on the deviated trajectory rather than on the average {110} glide plane. This new law agrees with both experimental and DFT measurements of Peierls stress variations with crystal orientation and enables understanding why Schmid law deviation is metal dependent. We can now predict Schmid law deviation in all BCC crystals from simple atomistic calculations and explain this well-known property characteristic of BCC plasticity.

(G1 oral) **Interaction of interstitial iron with dislocations in silicon**

B Ziebarth, M Mrovec, C Elsässer and P Gumbsch

Fraunhofer IWM, Germany

Dislocations play an important role in semiconductor devices made of crystalline silicon. They are known to be strongly performance-limiting defects in solar cell applications, since they act as preferred segregation sites for metallic impurities. In this work, we investigate the segregation of interstitial iron impurities at dislocations in Si, both at dislocation cores and in the long-range stress fields around dislocations, using atomistic calculations based on first-principles density functional theory. Our simulations show that interstitial Fe impurities segregate readily to all investigated cores and the driving force for the segregation increases with impurity concentration. In contrast, the formation energy of neutral Fe interstitials in the vicinity of dislocations is almost unaffected by lattice deformations of the Si crystal up to strains of 5%. We will present systematic analysis of structural, electronic, thermodynamic and kinetic aspects associated with the Fe segregation at the most common dislocations in Si, and compare them with available experimental observations.

(G1 oral) **Stabilization of the screw dislocation hard core by interstitial solutes in body-centered cubic metals**

B Luthi[1], L Ventelon[1], D Rodney[2] and F Willaime[1]

[1]CEA, France, [2]ILM - Universite Lyon, France

The core structure of screw dislocations in pure BCC metals has been the object of extensive studies and debates for several decades. Thanks in particular to DFT calculations, there is now a general consensus that the dislocation core adopts in pure metals the symmetrical easy core configuration. The other core configurations – the asymmetric core, the hard core and the split core – are all unstable in pure BCC metals. In this work, we investigate the effect of interstitial solute atoms on the ½ screw dislocations in BCC metals using ab initio calculations. First considering the case of Fe(C), our DFT calculations show that, when a row of solute atoms is added in the neighbourhood of the dislocation core, both the dislocation and the solute atoms reorganize towards a low-energy configuration, where, surprisingly, the dislocation adopts a hard-core configuration. The solute atoms are at the center of regular trigonal prisms formed by the Fe atoms inside the three core atomic columns [1], a local configuration similar to the building unit of cementite. We obtain the same core reconstruction with other solutes (B, N, O) in Fe and in other metals (W, Mo). NEB calculations show that the mobility of the transformed dislocations is very low. This agrees with recent in-situ TEM observations, which show that in the regime of dynamical strain ageing of steels, the mobility of screw dislocations is strongly reduced [2].

[1] L. Ventelon et al., Phys. Rev. B 91, 220102(R) (2015)
[2] D. Caillard, J. Bonneville, Scripta Mater. 95, 15 (2015)

(G2 invited) **Atomistic simulations of screw dislocations: core structure, Peierls potential, and finite temperature motion**

M Gilbert[1], J Marian[2] and S Dudarev[3]

[1]CCFE/Euratom, UK, [2]University of California, Los Angeles, USA

Dislocations are ubiquitous line defects that largely determine the response of a material to plastic strain. Therefore understanding of their behaviour is vital, particularly in nuclear applications where dislocations will occur in materials exposed to neutron irradiation, which will generate other defects and impurities that dislocations will have to overcome as they move. In materials with body-centred cubic (bcc) structure, screw dislocations govern the plastic behaviour at medium to low temperatures due to the thermally-activated character of slip. This makes them the central object of study for important structural materials based on, e.g., Fe or W.

Atomic simulations and modelling is one of the main ways of investigating the behaviour of screw dislocations because they can be performed in carefully controlled ideal scenarios and can thus be used to understand fundamental properties. This contrasts with, for example, experiments, where screw dislocations will be typically observed and investigated in materials with minor impurities or other lattice defects.

Over the last few years, there have been several significant advancements in the understanding of screw dislocations in important bcc metals. This paper will describe some of those recent advances, including how the correct core structure can be investigated and guaranteed in simulations; how the velocity of motion of screw dislocations changes with temperature and stress in massively parallel atomistic simulations; and how the energy landscape through which a screw dislocation travels by elementary kink processes can be calculated using thermodynamic integration techniques, revealing how it is changed by external factors.

(G2 oral) **Kink pair production and dislocation motion**

S Fitzgerald

University of Oxford, UK

Under moderate applied stresses, dislocations move through the periodic Peierls potential via the thermal nucleation of kink pairs. The nucleation rate, and hence the dislocation velocity, is an extremely nonlinear function of the applied stress and temperature. Previous theoretical calculations of the rate either involve computer simulations at the atomic scale (which are too computationally demanding for modelling plasticity) or produce approximate formulae (valid only for small or large applied forces). In this talk I will derive a simple, general, and exact formula for the rate, directly from the stochastic equation of motion for the dislocation, using methods drawn from quantum field theory. This formula fits experimental and numerical data very well, and also applies to the many other physical systems modelled by elastic strings interacting with periodic potentials. Consequences for microstructural evolution will be discussed.

(G2 oral) **Onset of plasticity in zirconium in relation with hydrides precipitation**

L Pizzagalli[1], W Szewc[2], S Brochard[2] and E Clouet[3]

[1]Institut P' / CNRS, France, [2]Institut P' - CNRS - Université de Poitiers, France, [3]CEA/DEN/SRMP Saclay, France

Hydride precipitation is a known phenomenon occuring in zirconium in the context of nuclear applications. It is an important issue since it severely degrades the mechanical properties of the material. Microscopy observations revealed that the hydride formation induces a plastic deformation of the Zr matrix, starting from the Zr/Zr-H interface. However, little is known about the initiation of plasticity in an hexagonal material like zirconium. In this work, molecular dynamics simulations were performed to investigate such a mechanism in zirconium, in conditions associated with the formation of hydrides. We considered the uniaxial deformation of a Zr slab, as well as the effect of a growing cylindrical cavity inside the material. These simulations show that plasticity is always initiated by the nucleation and propagation of pyramidal partial dislocations from the surfaces, followed by the formation of basal dislocations in a second step. This result is shown to be weakly dependent on several parameters such as surface orientation and roughness, loading conditions, temperature, and interatomic potential. Our analysis based on generalized stacking fault surfaces suggests that the favoured activation of pyramidal slip is related to a surface nucleation effect. Finally, the computed elasticity limits are in agreement with the strains associated with the formation of hydride precipitates.

(G2 oral) **Dislocation core transitions in disicides**

V Paidar[1] and M Šob[2]

[1]Institute of Physics AS CR, Czech Republic, [2]Masaryk University, Czech Republic

Due to several metastable stacking faults in the tetragonal $C11_b$ structure of $MoSi_2$ and a large number of possible dislocation splitting into partial dislocations, complex behaviour of mechanical properties is observed. Plastic deformation is controlled by several types of dislocations. Three types of dislocations (<100], 1/2<111], 1/2<331]) can be activated and their motion is directly related to their core configurations. Our analysis is based on the ab initio calculations of γ-surfaces for generalized stacking faults. Possible transitions of the static equilibrium dislocation core structures into mobile configurations will be discussed.

(G2 oral) **Multiscale modelling of dislocation loops and precipitates in irradiated metals**

A Lehtinen[1], F Granberg[2], L Laurson[1], K Nordlund[2] and M Alava[1]

[1]Aalto University, Finland, [2]University of Helsinki, Finland

Plasticity in crystalline materials is due to motion of crystal defects known as dislocations. Discrete Dislocation Dynamics (DDD) is method where the dislocations are modelled as straight segments connected by discretization points. Their long range stress fields is obtained from linear elasticity theory but the reactions related to the dislocation core, such as junction formation and pinning to defects require input from more microscopic approaches. This is especially important when modelling irradiated metals which may contain different radiation-generated point-like defects like precipitates. Besides point defects, radiation also creates dislocation loops. These two defect types serve as obstacles to dislocation motion and are the main reason behind radiation hardening, which has important implications in engineering applications like in designing structural parts of nuclear reactors.

We have developed a multiscale framework which combines Molecular Dynamics (MD) simulations into the DDD code ParaDis. In this framework we use MD to model dislocation-precipitate interactions and use the obtained parameters as an input in our new DDD precipitate model [1]. In the next stage of this work we add dislocation loops into the mix. The hardening features of the dislocation-precipitate-loop system is then investigated with large scale DDD simulations.

[1] Arttu Lehtinen, Fredric Granberg, Lasse Laurson, Kai Nordlund, and Mikko J. Alava."Multiscale modeling of dislocation-precipitate interactions in Fe: From molecular dynamics to discrete dislocations" Phys. Rev. E 93, 013309

(G3 invited) **Direct atomistic simulations of bulk crystal plasticity**

V Bulatov[1], L Zepeda-Ruiz[1], A Stukowski[2] and T Oppelstrup[1]

[1]Lawrence Livermore National Laboratory, USA, [2]Technische Universität Darmstadt, Germany

Dislocations are ubiquitous in metals where their motion presents the dominant and often the only mode of plastic response to straining. Over the last 15-20 years computational prediction and understanding of fundamental dislocation mechanisms of plastic response in metals has been in the crosshairs of the materials modeling community. The typical multiscale approach relies on atomistic molecular dynamics (MD) simulations to obtain dislocation mobility functions and local evolution rules that are then employed in mesoscale dislocation dynamics (DD) simulations to model crystal yield, flow, and hardening from the underlying dislocation motion. Here we present first direct atomistic MD simulations of bulk crystal plasticity that skip the DD mesoscale altogether and compute plasticity response of single crystal tantalum while tracing the underlying dislocation behaviors in all atomistic details.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

(G3 oral) **Molecular dynamics investigation of dislocation-dislocation interaction at Ag precipitate interface embedded in Cu matrix**

D Rapp, S Hocker and S Schmauder

IMWF, Universität Stuttgart, Germany

Due to the large difference in lattice spacing's in the Ag-Cu system, the interface of Ag-precipitates is covered by a dense network of misfit dislocations. In this work the interaction between a single edge dislocation and differently shaped Ag-precipitates is investigated by molecular dynamics shear tests. Each investigated particle is placed in the glide plane of this edge dislocation, which is forced to pass the particle by prescribing shear deformation on the system.

On its way through the particle, the dislocation is twice forced to interact with the misfit dislocations found at the precipitate interface, resulting in dislocation-dislocation reactions. Depending on the local misfit dislocation configuration the maximum shear stress observed in the glide plane (the critical resolved shear stress, CRSS) can be influenced significantly, resulting in local deviations from the usually observed linear scaling of the CRSS with precipitate diameter divided by spacing (D/L) found in coherent material systems for the case of dislocations cutting through a particle.

The results from such shear test are usually used to calibrate dislocation dynamics simulation, which then are able to predict the hardening caused by precipitate fields. The test is performed for spherical and octahedral particles, as well as for particles with intermediate shape which have been experimentally observed in investigations of Ag-Cu.

(G3 oral) **Evolution of dislocations during nanoindentation and nanoscratching of HCP metals: Molecular dynamics study**

I A Alhafez[1], Carlos Ruestes[2], Yu Gao[1] and H Urbassek[1]

[1]University Kaiserslautern, Germany, [2]Universidad Nacional de Cuyo, Argentina

Using molecular dynamics simulation, we study the nanoindentation of three hcp metals: Mg, Ti, and Zr. Both the basal and two prismatic surface planes are considered. We focus on the characterization of the plasticity generated in the crystal. The similarities to, and the differences from, the behaviour of the more commonly investigated fcc and bcc metals are highlighted. We find that hcp metals show a larger variety than the fcc and bcc metals studied up until now. The prolific emission of prismatic loops can lead to extended plastic zones. The size of the plastic zone is quantified by the ratio f of the plastic zone radius to the radius of the contact area. We find values of between 1.6 and >5; in the latter case, complex dislocation networks build up which are extended in the direction of easy glide.

In addition we explore scratching of Ti and Mg crystals. Both basal and prismatic surface orientations are considered. Among the various types of dislocations generated the partials 1/3 are most prominent. Plastic activity is more pronounced for the prismatic surface. Under the basal surface intrinsic stacking faults are formed parallel to the scratch groove bottom, while they are oriented perpendicular to the surface under the prismatic surface. We find that mainly the {01-10} slip system is activated, and relate the form of the pile-up generated to this slip. The tangential hardness is systematically smaller than the normal hardness under scratching. The basal surface has smaller hardness than the prismatic surface.

(G3 oral) **Molecular dynamics simulations of intrusions and extrusions in iron, copper and nickel during cyclic loading**

Y Maniar[1], P Binkele[2], A Kabakchiev[1] and S Schmauder[2]

[1]Robert Bosch GmbH, Germany, [2]University Stuttgart, Germany

Lifetime prediction in structural metallic components is often a challenging task due to the complex mechanisms of crack initiation and fatigue. Cyclic loading in metallic materials lead to dislocation movement and thus, to localized plastic deformation. The sliding processes in the crystal lattice are depend on both the bulk-material properties and near-surface defects. Dislocations often transform into persistent local slip bands (PSB), which move along preferred crystallographic planes. Under shear stress PSBs slip towards the surface where they can form intrusions and extrusions. This leads to a roughening of the sample surface and is assumed to be the precursor of nano-scale cracks. However, the irreversible surface modifications on the atomic scale is still not completely understood. In this work, the beginning of fatigue failure in the form of intrusions and extrusions is examined in detail by means of molecular dynamics (MD) simulation. We analyse the surface deformations by MD-simulations of cyclic tension-compression loads on nano-scale single crystal models of Fe (bcc), Cu (fcc) and Ni (fcc). The influence of lattice structure, crystal orientation, strain rate and crystal defects on the intrusion and extrusion formation is examined and discussed. The present results reveal the mechanisms preceding crack initiation at the atomic scale, providing a deeper understanding of metal fatigue under cyclic mechanical loads.

(G4 invited) **Recent progress in dislocation dynamics simulation and its contribution to crystal plasticity modelling**

B Devincre

LEM, CNRS-ONERA, France

Since the first MMM conference in 2002, dislocation dynamics (DD) simulations have always been a symbol of multiscale investigations in material science. DD simulation is today a well establish numerical method, filling a strategic gap existing at the mesoscopic scale between atomistic simulations focussed on dislocation core properties and continuum models devoted to the calculation of mechanical properties at larger scales. Here, we present some recent progresses made in the context of collaborations using the popular lattice based DD simulation code, "microMegas".

This review will cover technical and theoretical aspects associated with the local rules used in the simulations to reproduce dislocation core properties and the calculation of elastic properties. Applications of the DD simulations to important current topics like - the identification of more physically justified parameters for crystal plasticity models, - the study of strain hardening mechanisms involved in materials deformed with complex loading, - the origins of size effects in nanomaterials and nanostructures and - the dynamics of plastic zone at crack tip will be presented.

(G4 oral) **The interaction strengths between slip systems revisited**

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The Mobile Dislocation Colony (MobiDiC) dislocation dynamics simulation code was used to revisit dislocation strengthening for a selection of metallic single crystals. Complex slip geometries can be handled. The code also includes a careful treatment of the line tensions at the triple nodes of junctions and is well suited for extensive studies on large clusters. Making use of the average isotropic shear moduli and Poisson's coefficient proposed by Scattergood and Bacon improves the quality of the numerical results.

For example, in the case of BCC metals, MobiDiC incorporates {110} and {112} slip systems and routinely allows thousands of processors to be used in order to develop a comprehensive study of the interaction coefficients between slip systems.

The results are discussed in terms of two effects that have not been investigated as yet. The first one is the effect of the effective Poisson coefficient on the strength of dislocation reactions and the second one is the double degeneracy of some interaction coefficients when the active and forest slip systems are exchanged. Preliminary results on the coefficients that determine the dislocation mean free paths will also be discussed.

These investigations are part of an ongoing work on a generalized storage-recovery model for strain hardening in BCC metals at high temperatures.

(G4 oral) **Plastic zone properties at a crack tip investigated with the Discrete-Continuous Model**

L Korzeczek[1], R Gatti[2], A Roos[3] and B Devincre[2]

[1]ONERA, France, [2]LEM [ONERA/CNRS], France, [3]SAFRAN TECH, France

In this study, the dynamics of dislocations inside the plastic zone formed at the vicinity of trans-granular short cracks is investigated at the mesoscopic scale with the Discrete-Continuous Model (DCM). The results of this model, based on a coupling between 3D Dislocation Dynamics and Finite Elements simulations, are here presented and compared with a conventional Crystal Plasticity Model (CPM) appropriately set up to correctly reproduce slip system interactions in FCC single crystals.

Several crack orientations were studied for single or polycrystal materials, under monotonous or cyclic loading. A detailed analysis of the respective slip system activity around the crack in relation with shielding and blunting mechanisms is presented. To calculate the 3D strain energy release associated to plastic deformation and controlling crack propagation, a G-theta integral method is used and compared with alternative local force solutions. Also, the strong differences observed between the DCM and the CPM simulations are systematically analysed and discussed. These results are of particular interest for the development of more physically justified dislocation density based model devoted to fracture problems in ductile materials.

(G4 oral) **Modeling the bauschinger effect and cyclic hardening in single crystals from dislocation dynamics simulations**

S Queyreau[1] and B Devincre[2]

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Bauschinger Effect (B.E.) is defined from simple forward and reverse loading tests, and is manifested by the reverse flow curve exhibiting a reduced elastic limit, a well-rounded appearance of the initial plastic section and a permanent softening with respect to a continuous forward hardening curve. Investigation of B.E. is of particular interest for the understanding of cyclic deformation and for the modelling of kinematic hardening in crystal plasticity. Today, existing interpretations of the B.E. and cyclic hardening are dominated by phenomenological model that are based on the concepts of long-range internal stress (back stress) and/or easy glide at strain reverse induced by partial microstructure dissolution. However, such interpretations are in many regards not consistent with the B.E. observed in single crystals.

In this study, the B.E. of Ni and Cu single crystals is investigated with the help of 3D dislocation dynamics simulations. Among the different elementary features controlling the strain hardening, we show that the junction strength and the mobile dislocation mean free path are key physical parameters to understand the dislocation microstructure asymmetry upon load path changes. A new model based on the short-range properties we observed in DD simulations is proposed. This model, whose parameters are directly calculated from simulations, captures quantitatively many details of existing experiments on Baushinger and cyclic loading in single crystals.

(G5 invited) **Large scale dislocation dynamics simulations of plasticity and point defect evolution in persistent slip bands**

J El-Awady[1] and A Hussein[2]

[1]Johns Hopkins University, USA, [2]Air Force Research Laboratory, USA

One of the common dislocation microstructures forming during cyclic loading of face centered cubic metals are persistent slip bands (PSBs). Over the years, many experimental, theoretical, and computational studies have led to significant understanding of plasticity in PSBs, however, many open questions still remain in the prediction of the formation and evolution of these complex dislocation structure. In this work, large scale three-dimensional (3D) discrete dislocation dynamics (DDD) simulations are performed to study dislocation plasticity and point defect evolution in PSBs in single-slip oriented nickel single crystals. In these simulations partially developed PSB structures are introduced into the simulation cell and fully reversible loading is imposed. The maximum stress of the hysteresis loops and the local dislocation density in the channels/walls are shown to increase with increasing loading cycle. The dislocation interactions in the channels and the 3D contours of the local shear stress within the channels as a function of distance from the PSB walls are characterized to re-evaluate the composite model proposed by H. Mughrabi and the bowing and passing model by L.M. Brown. In addition, the spatio-temporal point defect (vacancies and interstitials) generation and evolution is quantified as a function of the dislocation density in the PSB channels and walls. The results are discussed in view of a point defect diffusion model to study their migration rates to the surface. Finally, the PSB interaction with the free surface and the surface roughness evolution are also quantified.

(G5 oral) **Strain bursts and dislocation avalanches in irradiated micropillars**

N M Ghoniem, Y Cui and G Po

University of California, Los Angeles, USA

Experiments on the yield and plastic hardening of submicron specimens have revealed strong statistical variations from experiment-to-experiment. When materials are subjected to ion or neutron irradiation, defect clusters are produced, and result in strong interactions with dislocations. In fcc metals, stacking fault tetrahedra and slef-interstitial atom clusters impeded dislocation motion. Likewise, dislocations are immobilized by nano-voids and interstitial clusters in bcc metals. Recent experiments indicate that the yield strength is increased by irradiation, and that the statistical distribution of strain bursts and associated dislocation avalanches also change. We present here a computational study of plastic deformation of irradiated and unirradiated submicron specimens subjected to an externally applied constant stress or displacement rates. These two conditions show distinct plastic response characteristics. Dislocation avalanches result in strain bursts under conditions of constant stress rate, and in stress relaxation bursts under constant strain rate conditions. The statistics of strain and stress relaxation bursts are shown to obey general scaling laws, limited by the size of the submicron specimen. We present results of 3-D Discrete Dislocation Dynamics (DDD) simulations, based on our code for the Mechanics Of Defect Evolution Library (MODEL). The results are analysed to yield information on the frequency distribution functions of strain bursts, auto-correlation between bursts, and scaling exponents. Scaling laws based on the distribution functions of strain and energy bursts are given. We derive scale-free power laws for such bursts caused by dislocation avalanches, and present a study of the nature of self-organized criticality demonstrated in irradiated and unirradiated materials.

(G5 oral) **DD simulations of interactions between gliding dislocations and radiation-induced loops in α-iron: bridging the atomic and the crystalline scales**

X Shi[1], L Dupuy[2], B DEVINCRE[3], D Terentyev[4] and L Vincent[2]

[1]Université Paris 13, France, [2]CEA, France, [3]CNRS-ONERA, France, [4]SCK-CEN, Belgium

The mechanical behaviour of iron-based steels under neutron irradiation at moderate to high doses is mainly influenced by the presence of radiation defects such as dislocation loops. A strategy of multiscale modelling from the atomic scale to the microstructure scale has been set up within the European PERFORM60 project to study the hardening produced by the interaction between these loops and mobile dislocations.

Based on the elementary interaction mechanisms between loops and gliding dislocations determined at the atomic scale from Molecular Dynamics simulations (MD), we systematically reproduced in a qualitative and quantitative manner the elementary features controlling irradiation hardening with the Dislocation Dynamics (DD) code Numodis. Various configurations with different dislocation characters and different types of loops were considered. The remarkable correspondence we obtained between MD and DD simulations shows that DD simulation is a powerful method to analyse and extend our understanding of the complex features observed in atomistic simulations.

DD simulations were then performed on larger systems, approaching more realistic experimental configurations, to investigate the effect of loop density, size distribution and applied strain rates. Results of these simulations provide useful information about collective processes involved in irradiation hardening for upper-scale models such as the Crystal Plasticity Finite Element Method (CPFEM).

(G5 oral) **The effect of temperature and dislocation mobility on the attenuation of the dynamic yield point in shocks**

B Gurrutxaga-Lerma, D Balint, D Dini, A Sutton and D Eakins

Imperial College London, UK

The attenuation of the dynamic yield point in shocked materials, otherwise known as the elastic precursor decay, is a fundamental feature of the dynamic behaviour of shocked metals; the elastodynamic fields of dislocations generated at the front have an accumulated shielding effect that explains the yield point's attenuation. Experimental studies show that the magnitude of the attenuation is a function of the temperature of the system, and depending on the material and the strain rate, the dynamic yield point may increase or decrease with temperature. This is because temperature affects both the mobility of dislocations, the different dislocation generation mechanisms, and the the value of the elastic constants which dominate the response of the system. In this talk, we employ Dynamic Discrete Dislocation Plasticity (D3P), the elastodynamic extension of discrete dislocation dynamics, to explore the effect temperature and mobility laws have on the dynamic response on a number of metals, offering an explanation to the experimentally observed temperature dependence affecting the dynamic yield point.

(G5 oral) **A discrete dislocation dynamics description of grain boundary sliding and its contribution to plastic deformation in polycrystalline materials**

S S Quek[1], Y W Zhang[1] and D Srolovitz[2]

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Grain boundaries (GBs) play significant roles during the deformation of polycrystalline materials. We know that GBs in metals consist of repeated atomic structures and defects (like dislocations and steps). These characteristics means that they can do more than obstruct lattice dislocation motions. Reactions of GBs with lattice dislocations occur, which can result in absorption, nucleation and transmission of dislocations at the GBs. In addition, GBs also migrate and serve as surfaces where grains slide against one another. These mechanisms contribute synergistically with one another to the overall deformation of a polycrystalline metal, even though the extent of their individual contribution can vary depending on factors like grain size, temperature, material system, and so on. While the discrete dislocation dynamics method has been very successful in accounting for plastic slip during deformation, when applied to a polycrystalline system, GBs have conventionally been treated as mere obstacles to dislocation motion, and other mechanisms associated with GBs have very often been neglected. In this work, we describe athermal GB sliding by the glide of GB dislocations along the GB using the discrete dislocation dynamics method, and show that when coupled with lattice dislocation emission at GB junctions, it can recover the inverse Hall-Petch relation when grain sizes are in the nanoscale regime. We also discuss how the model can be extended beyond athermal GB sliding to account for shear-coupled GB migration.

(G6 invited) **Continuum dislocation modelling of wedge indentation**

G Po and N Ghoniem

University of California, Los Angeles, USA

Recent EBSD experiments have revealed the heterogeneous dislocation microstructure forming under a wedge indenter in fcc crystals, where micro-meter dislocation patterns challenge the predictions of traditional models of plasticity. In order to explain the formation of these features, in this work we present a model of wedge indentation based on the continuum theory of dislocations. The model accounts for large deformation kinematics through the standard multiplicative split of the deformation gradient tensor, where the incompatible plastic component of deformation results from the flux of dislocations on different and interacting slips systems. Constitutive equations for the dislocation fluxes are determined from a dissipative variational principle given two thermodynamic potentials. As a result, each dislocation density satisfies an initial-boundary value problem with convective-diffusive character, which is coupled to the macroscopic stress-displacement problem governing the deformation process. Solution to the self-consistent continuum formulation is found using the finite element method. In particular, computer simulations are performed for cases that mimic the experimental conditions used in wedge micro-indentation experiments of fcc Cu, Al, and Ni. A comparison of overall dislocation density distribution and macroscopic mechanical response is presented.

(G6 oral) **Dislocation multiplication and cross-slip in continuum dislocation dynamics**

T Hochrainer[1], A Ebrahimi[1] and A El-Azab[2]

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Within the last years, continuum dislocation dynamics (CDD) has been turned from a kinematic concept to describe moving curves into a statistical continuum theory of dislocations. However, CDD is as yet mostly developed for single slip, when dislocation multiplication is driven by loop expansion without creating new loops. This restricts the applicability of CDD to small scales and moderate strains, while the most conspicuous feature of plastic deformation, i.e. work hardening, is not covered.

Work hardening is traditionally discussed in terms of the dislocation ‘mean free path’, which really is the inverse of the dislocation line-length produced per area swept. In CDD this corresponds to the average radius of curvature, defined through the quotient of dislocation density and curvature density. Dislocation multiplication for CDD henceforth is mostly a matter of a source term in the evolution of the curvature density. The key to a model of dislocation multiplication is consequently a coupling of the dislocation curvature evolution to dislocation junctions or jogs and to points where dislocations change glide plane, as in the case of cross slip.

In the current contribution we present kinematic descriptions for dislocation multiplication and cross-slip. The evolution is coupled to the current dislocation state using data from discrete dislocation simulations. The resulting theory is incorporated in a CDD-based crystal plasticity materials law implemented in a finite-element solver. Using these multiplication laws we are able to predict the turnover from bulk plasticity to surface dominated starvation observed in micro-pillar compression tests when decreasing the pillar size.

(G6 oral) **Phase-field modelling of dislocations in face-centered cubic materials involving micropores**

A Ruffini[1], A Finel[2] and Y Le Bouar[2]

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In material science, one of the ubiquitous difficulties is to describe the development and evolution of mesoscale microstructures whose properties are closely controlled by phenomena requiring a microscale description. For example, single-crystal nickel-based superalloys used in aerospace industry can exhibit micropores acting as potential sources of fatigue failure. The pores can be removed by hot isostatic pressure (HIP). The problem is to model the physics of the pore annihilation since it involves a wide variety of mechanisms which themselves stand at a much lower scale (dislocations, microcracks…) [1].

Numerically, in strategies consisting in describing some of these processes, atomistic simulations usually fail to account for realistic systems with high enough space and time scales. Continuum methods, such as the phase-field thus appear as potentially well adapted alternatives. To this end, we have recently proposed a new phase-field model to explicitly couple individual cracks and dislocations [2]. Notably, this model allows us to consider the physical entities at their characteristic time scale, in a numerical formulation that enables the management of complex free surfaces.

In this presentation, the actual model extended to the face-centered cubic geometry will be exposed and illustrated in the context of pore annihilation by plastic flow in single-crystal nickel-base superalloys. Particular attention should be paid to the competition between plasticity and surface energy on the morphology of nanopores.

[1] A. Epishin et al., Mater. Sci. and Eng. A, Vol. 586 (2013) pp. 342-349.
[2] A. Ruffini, A. Finel, Acta Mater., Vol. 92 (2015) pp. 197-208.

(G6 oral) **Atomistic simulation of face-centered cubic metallic nanospheres under uniaxial compression**

S Bel Haj Salah, C Gerard and L Pizzagalli

Institut Pprime, France

The mechanical response of metallic nanoparticles appears to be of a special interest due to their specific properties compared to their bulk counterpart. Nevertheless, these kind of nano-objects have been much less investigated than other low-dimension systems like nanowires and nanopillars. To improve our current understanding in this domain, molecular Dynamic simulations have been carried out to study the uniaxial compression of face-centered cubic metallic (FCC) spherical nanoparticles. EAM potentials were used to describe the interatomic interactions in Al, Ni, and Cu. We investigated how the mechanical behaviour depends on several parameters such as nanoparticles size, compression orientation, and temperature. First, we present results related to the elastic domain, with a focus on the elastic modulus associated to compression. Then the plastic deformation mechanisms are analysed in details. In all cases, partial dislocations nucleate at the top and bottom contact edges of the nanosphere, followed by their propagation throughout the nanoparticle. Depending on the crystallographic orientation of the nanoparticle, the nucleation process may also include the temporary formation of a pyramid hillock structure. The three tested FCC metals allowed us for studying the effect of different stacking fault energies (SFE). We found that deformation mechanisms switched from a dislocation slip-dominant regime to a twin-dominant regime when the SFE is lowered, as expected.

(G7 invited) **Continuum dislocation dynamics: From dislocation kinematics to work hardening**

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Continuum dislocation dynamics represents the stress-driven motion of dislocation lines in a density-based framework, accounting for dislocation transport and dislocation interactions. Here we discuss for the simplest possible case - a statistically homogeneous and isotropic dislocation system - how this framework can be generalized to account for dislocation multiplication (generation of new loops) and annihilation. We formulate the elastic energy functional of the dislocation system in terms of the dislocation densities, identify energy contributions that are dissipated and that are stored during plastic fow, and investigate the resulting work hardening behaviour. In particular, we demonstrate that the CDD framework naturally accounts for both transient and permanent changes in flow stress subsequent to a strain path change. The model is parameterized by reference to macroscopic hardening curves of Cu single crystals and validated by investigating the associated Bauschinger effect.

(G7 oral) **Modelling the creep properties of olivine in the lithospheric mantle from dislocation dynamics models**

K Gouriet[1], F Boioli[2], B D Devincre[3], P C Carrez[1] and P Cordier[1]

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Large scale flow in the Earth’s mantle involves plastic deformations of rocks and their constitutive minerals. Due to the extremely slow strain rate conditions in the Earth's mantle, it is very challenging to identify the fundamental mechanisms controlling such process. Thus, the development of a multi-scale approach linking the atomic scale properties and the microscopic elementary mechanisms to the macroscopic behaviour is needed [1]. One of the key step in this approach, is the description of dislocation-based intra-crystalline plasticity. Within this framework, we present a model to investigate the creep of olivine, one of the main constituent of the Earth's mantle, at the mesoscopic scale. In particular, we employ 2.5-Dimensional (2.5-D) dislocation dynamics simulations to investigate the interplay between thermally activated glide and climb [2,3] and/or cross-slip motion and to study the effect of climb and/or cross-slip on olivine creep strain rates .

In this study, we performed simulations in steady state creep conditions on the temperature between 800 K and 1700 K, and we applied creep stresses between 10 and 100MPa. In these ranges of temperature and applied stresses, we investigate the role in plastic behaviour of both slip system [100](001) and [001](100) and of the both thermally activated mechanisms.

[1] P. Cordier et al., Nature 481, 177 (2012)
[2] Boioli et al., Phys. Rev. B. 92, 014115 (2015)
[3] Boioli et al., EPSL. 432, 232 (2015)

(G7 oral) **An accurate and efficient elastic force computation for discrete dislocations in anistropic polycrystals**

A Arsenlis[1], S Aubry[1], E Tarleton[2], S Queyreau[3], J Knap[4], L Munday[4], J Crone[4], M Rhee[1] and B Liu[1]

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The next frontier for discrete dislocation dynamics is the simulation of discrete plasticity in polycrystalline aggregates. As with the simulation of single crystals, the largest barrier to overcome in the simulation of discrete dislocation plasticity in polycrsytals is one of computability, and in particular the accurate and efficient computation of forces acting upon the dislocation microstructure. The forces arise due to dislocations interacting with dislocations within their own grain, with dislocations in other grains, and with the externally applied loads. For elastically isotropic polycrystals, the computation of forces can follow the accurate and efficient computational methods developed for single crystals, but for elastically anisotropic polycrystals those methods breakdown because the elastic Green's function can no longer be used across grain boundaries. Techniques have been proposed to overcome this limitation by coupling the Green's function methods with finite element or other field solution methods, but none have ever been evaluated for their accuracy and computational cost, and some of the simplest proposed methods are also the most computationally expensive. In this talk, we will evaluate many of the proposed computational methods for their accuracy and efficiency, and propose a new one which uses and analytical approximation to the anisotropic Green's function for the computation of elastic interactions between dislocations in the same grain, and uses finite elements for the computation of elastic interactions between dislocations in different grains. Furthermore, the communication between the two field solution methods requires only local communication in the simulation volume with added communication at grain interfaces.

(G7 oral) **Atomistically based discrete dislocation dynamics simulations of plastic deformation in Magnesium**

K Srivastava and J El-Awady

Johns Hopkins University, USA

Plasticity in magnesium crystals oriented for c-axis compression is usually attributed to <c+a> dislocation slip on pyramidal planes. So far in discrete dislocation dynamics simulations, the mobility of dislocations on pyramidal slip planes has been assumed to be isotropic. Recent systematic molecular dynamics studies clearly show that the edge <c+a> dislocations are immobile on the pyramidal I planes, while the screw dislocations are highly mobile and have low critical resolved shear stresses. Furthermore, the mobility on pyramidal II planes is significantly harder with high Peierls stress. Here, we present 3D discrete dislocation dynamics simulations accounting for the anisotropy of pyramidal slip in Mg as computed from molecular dynamics simulations. Large-scale c-axis compression simulations of different Mg crystal sizes are conducted and the dislocation microstructure evolution in both bulk and small-scale samples is thoroughly investigated. The results are compared with recent transmission electron microscopy from deformed Mg single crystals.

(G7 oral) **Parametric model of double cross-slip treated by mathematical theory of evolving curves**

M Kolář, M Beneš and J Kratochvíl

FJFI CVUT v Praze, Czech Republic

In this contribution we analyse the problem of dislocation cross-slip considered as a deterministic, stress-driven elementary dislocation process. Our approach to modelling the dislocation dynamics is based on mathematical theory of smooth curves evolving either in plane or on a two dimensional surface. The motion of dislocation curves is driven by the mean curvature motion law in the form

$B\,v = T\,\kappa + F.$

Here v denotes the normal velocity, F is the normal component of all external forces acting on the dislocation, and parameters B and T denote the drag coefficient and the line tension, respectively. In the case of planar curves, the κ is the mean curvature, and in the case the dislocation evolving on a surface, κ stands for geodesic curvature.

The cross-slip is considered as a deterministic phenomenon controlled by the repulsive exerted by a spherical obstacle. The sharp edges between the primary planes and the cross-slip plane are regularized to ensure the C^2 smoothness of the whole glide surface. For numerical simulations, we employ the parametric description of the evolving dislocation curves and semi-implicit flowing finite volume method. To ensure the numerical stability, the employed semi-implicit scheme is enhanced with the tangential redistribution of the discretization points. Overcoming of a spherical obstacle by double cross-slip is presented as an illustrative example. The results of computational experiments are compared with the results obtained by the established projection method.

(G8 invited) **Solid solution hardening in Fe-X alloys (X=Si, Ni, Al, Cr)**

D Caillard

CEMES-CNRS, France

Alloying iron with various substitutional atoms induces a strong hardening close to room temperature, which can be interpreted in terms of a Cottrell interaction between dislocations and immobile solute atoms. Which dislocations (screws or edges) are responsible for this hardening remains however unclear. Indeed, the Cottrell interaction is generally assumed to be the strongest on edge dislocations, whereas the plasticity is controlled by the velocity of screw dislocations below room temperature. An inversion between the relative velocities of edges and screws could thus be expected at some transition temperature.

In order to determine the exact origin of solid solution hardening, in situ straining experiments at low temperature have been carried out in a JEOL 2010 transmission electron microscope, in pure Fe and in various binary FeNi, FeSi, FeCr and FeAl alloys.

The results show that screw dislocations always remain the less mobile ones. Under such conditions, solid solution hardening does not result from a classical Cottrell interaction, but from the pinning of screw dislocations at super-jogs formed by cross-slip in the vicinity of substitutional solute atoms. The corresponding amount of stress increase has been clearly correlated to the density of pinning points and to the concentration of solute atoms. When expressed in terms of a simple line-tension model, it fits fairly well to that measured in mechanical tests.

(G8 oral) **Cross-slip in FCC solid solutions**

W Nöhring and W A Curtin

École Polytechnique Fédérale de Lausanne, Switzerland

Many engineering alloys contain a significant concentration of substitutional solutes. Understanding how these solutes affect dislocation motion, and macroscopic plastic behaviour, is required for developing predictive models of alloy strength. Here, the role of solutes on dislocation cross-slip is studied in fcc crystals. According to the Friedel-Escaig model, the activation energy for cross-slip depends on the elastic constants and the stacking fault energy, and so one might imagine that solute effects are confined to solute dependence of these quantities. However, since cross-slip is initiated by a nucleation process, it can be sensitive to local concentration fluctuations. To demonstrate that cross-slip is controlled by such fluctuations, large-scale molecular statics calculations have been used to compute the cross-slip transition path in NiAl and AlMg solid solutions and in the corresponding "average" alloys using an "average atom" interatomic potential. The average alloys have the same average properties as the true random solutions, but do not have local fluctuations. Results show that cross-slip is indeed governed by solute fluctuations. In other words, there are local arrangements of solutes that provide an activation barrier for cross-slip that is lower than the barrier in the average alloy, and cross-slip thus occurs preferentially at such local fluctuations. The local conditions causing the low activation barriers are analysed. The overall effect of solutes on the cross-slip rate of long dislocation lines, and in particular the scaling of cross-slip rates with solute concentration, is also discussed as well as the implications on macroscopic hardening and softening in solution-strengthened alloys.

(G8 oral) **A unified model for solid solution strengthening in high-entropy BCC alloys**

F Maresca and W Curtin

École Polytechnique Fédérale de Lausanne, Switzerland

BCC alloys are an important class of metals with technologically relevant applications. Plastic deformation is understood to be governed by the thermally-activated nucleation and propagation of kink-pairs along screw dislocations, as influenced by the interactions with the solutes resulting in either softening or strengthening. Models for this behavior exist (e.g. Suzuki 1979; Trinkle and Woodward 2005) that involve a number of assumptions and with a focus on moderate concentrations and one solute type.

We present a model for solid solution strengthening in random BCC alloys at arbitrary concentrations and for multiple species. The model first identifies that a straight dislocation line will become kinked immediately to take advantage of low-energy fluctuations in the local solute arrangements. A parameter-free expression for the yield stress of the alloy as a function of composition, temperature, and strain rate is obtained, and validated against experimental data and MD simulations. Limiting cases are considered, and similarities and differences with literature models are identified and discussed.

(G8 oral) **Atomistic modelling and time-series electron microscopy investigation of an elementary screw dislocation motion at a grain boundary in gold**

F Lançon[1], M Bowers[2], C Ophus[2], A Gautam[2], D Caliste[1] and U Dahmen[2]

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Cooperative atomic displacements at grain-boundary steps are observed by high resolution electron microscopy. Extended time sequences are recorded at a rate of 8 frames/s and structural events are detected by the correlation between pixel variations in the images. The cumulative averaging between these events produces very precise images of the successive states, with the possibility of following atomic rows displacements in 2D.

The goal is then to uncovered the mechanisms through molecular dynamics and other simulation techniques to get the 3D structures and the detail of the time evolution.

We show how one elementary mechanism involved in the grain boundary motion can be analyzed as the results of the motion of a screw dislocation associated with the step, i.e. a disconnection motion. Minimal-Energy path calculations for this event give the detail of the dislocation-core jump during the transition.

This mechanism is also spontaneously observed in a molecular dynamics calculation, though at a temperature set higher than the experimental one in order to accelerate the transition rates.

These calculations and the repeated observations imply that this mechanism is expected to have broad implications for thermally activated grain boundary migration.

(G9 invited) **Crystal plasticity simulations of the mechanical behaviour of Mg alloys**

J Segurado[1], V Herrera-Solaz[2], R Sánchez[3], J Molina-Aldareguia[3] and J Llorca[3]

[1]Polytechnic University of Madrid, Spain, [2]Paul Scherrer Institute, Switzerland, [3]IMDEA-Materials Institute, Spain

Crystal Plasticity models have been used to study the mechanical behaviour of Mg alloys, from the crystal level to macroscopic polycrystals. The work aims to understand the mechanisms responsible of the behavior of Mg crystals and polycrystals when deformed in both macro and microscopic tests.

At the microscale, nanoindentation of pure Mg grains was performed. The experiments were modeled using a CP Finite Element (FE) model. The set of Critical Resolved Shear Stresses that best reproduce the indentation tests in crystals under different orientation was obtained. In addition, the effect of indentation depth and temperature on twinning has also been studied.

At the macroscale, computational homogenization by means of the FE analysis of a Representative Volume Element of the microstructure is used to obtain the mechanical behavior. In order to obtain the parameters of the CP model, an inverse optimization technique based on the Levenberg-Marquardt method has been developed. The technique uses several independent macroscopic experimental curves to obtain the set of crystal parameters that produce the best agreement of the CPFE simulations with all the experimental data. The method was applied to three different alloys, and for each one tests at three different orientation were used. The resulting polycrystalline model accurately predicts tests independent to the ones used for fitting. Finally, the polycrystalline model has been applied to study the reverse yield asymmetry in Mg-rare earth alloys at high temperature. The model suggests the effect of non-Schmidt stresses and shear directionality in the activation and slip in pyramidal systems.

(G9 oral) **Intrinsic scale effects in the deformation of structural materials**

C Woodward[1], S Rao[2], A Hussein[1], E Antillon[3], B Adkim[3] and T Parthasarathy[3]

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There are several key deficiencies in current computational mechanics methods that need to be addressed in order realize the digital systems engineering (Integrated Computational Materials Science and Engineering). These issues include the need to homogenize material response without regard to material heterogeneities and the lack of an intrinsic length scale. Aspects of these issues can be addressed using a bottom up approach. Scale effects can be characterized, quantified and validated using lower scale, physics-based models that can be systematically verified experimentally. This can be used to develop scale dependent analysis methods to inform modelling of microstructure heterogeneities. Recent experiments have shown strong size effects in metal micro-pillars with dimensions below ~100 micro-meters. This size dependent behaviour is consistent with deformation occurring below a characteristic dislocation correlation length. Micro-scale dislocation evolution models of comparable micro-samples exhibit the same behaviour and were instrumental in determining the source of the strength and stochastic nature of this deformation. In this talk we review the results of large scale atomistic and dislocation dynamics simulations used to assess the aspects of ensemble hardening in simple metals. Large scale atomistic calculations illustrate the effects of cross slip on full 3-d simulations of forest hardening. The work hardening rates of micro pillars, uniaxial loaded along <100>, <110>, and <111>, are calculated using dislocation dynamics simulations. Simulations include dislocation intersection cross slip which enhances the rapid increase in dislocation density. Analysis of the evolving dislocation ensembles, including the formation of strong dislocation heterogeneities will be reviewed.

(G9 oral) **A multi-scale model of dislocation creep in MgSiO3 perovskite**

P Carrez[1], F Boioli[1], B Devincre[2] and P Cordier[1]

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The study of mechanical properties of minerals is of primary importance to model deformation and flow in the Earth's mantle which are responsible for plate tectonics and related phenomena. Numerical modelling provides an alternative to deformation experiments to address the behaviour of materials under extreme conditions, high temperature, high pressure and low strain rate. We propose a multi-scale model of creep behavior of MgSiO3 bridgmanite, a perovskite like silicate considered nowadays as the main constituent of Earth lower mantle. In this work, we rely on 2.5-dimensional dislocation dynamics simulations coupling climb with the glide dislocation motion to model the creep behaviour of MgSiO3 in high pressure conditions. In this multi-scale model, atomistic calculations of dislocation core properties, including kink-pair mechanism, are used to infer the glide velocity of dislocation used as an input of DD simulations. We show that by including the climb mechanism (where dislocations are sources and sinks for vacancy diffusion), we reach steady state creep conditions. We will further show that our calculations highlight the efficiency of pure climb creep compared to Nabarro-Herring creep. Therefore, pure climb creep provides a very efficient mechanism to account for flow at high-temperature in planetary interiors, even under very high pressures.

(G9 oral) **The role of climb in the plastic deformation of earth's materials: recovery process and viable strain producing mechanism**

F Boioli[1], B Devincre[2], P Carrez[3] and P Cordier[3]

[1]University of Lyon1, France [2]LEM, CNRS/ONERA, France, [3]UMET, Université Lille1, France

Dislocation climb is a key mechanism in the deformation of crystals. Although it is generally accepted that climb strongly affects dislocation microstructure and evolution at high temperature, the effect of climb on creep behaviour is still poorly known in many materials. Recently, creep power-law in Al has been successfully described by including climb in a dislocation dynamics (DD) model [1]. We expect climb to have a strong influence also on the plastic behaviour of materials characterized by high lattice resistance, such as olivine and other Earth's mantle minerals.

In this work we present 2.5-dimensional (2.5D) DD simulations coupling climb with the glide dislocation motion to model the creep behaviour of some important phases of the Earth's mantle. First, we employ this method to determine the creep strain rates in olivine, a mayor phase of the Earth's mantle. Climb emerges as a key recovery process that allows to attain steady state creep rates [2]. Moreover, we find a creep power-law in agreement with experimental results and we provide a model based on Orowan's law to predict the creep strain rates in the high temperature regime. Second, we show that, at geological strain rates, the interplay between glide and climb leads to steady state deformation conditions even at low/intermidiate temperatures [3]. Finally, we show that for some high-pressure phases characterized by an extremely high lattice resistance, dislocation glide is inhibited and climb can turn into an effective strain producing mechanism.

[1] Keralavarma et al. 109,265504,PRL(2012)
[2] Boioli et al., PRB. 92,014115(2015)
[3] Boioli et al., EPSL. 432,232(2015)

(G9 oral) **Unraveling the temperature dependence of the yield strength of tungsten single crystals using atomistically-informed crystal plasticity**

J Marian[1], D Cereceda[2], F Roters[3] and D Raabe[3]

[1]University of California Los Angeles, USA, [2]Johns-Hopkins University, USA, [3]Max-Planck-Institut für Eisenforschung, Germany

The plastic behaviour of BCC single crystals is governed by screw dislocation glide on close-packed crystallographic planes. Screw dislocation motion occurs via thermally-activated nucleation and relaxation of so-called kink pairs on a periodic energy substrate known as the Peierls potential. A long standing puzzle regarding BCC plasticity has been the discrepancy between the measured values of the yield/flow stress in tensile deformation tests and the calculated values of the Peierls stress at the atomistic scale. Here, we present a model that unifies both concepts and provides a justification for the differences in terms of the non-Schmid behaviour displayed by BCC crystals. Our model consists of a crystal plasticity microstructural engine parameterized entirely using atomistic calculations, that includes full non-Schmid effects as well as a physically-consistent flow rule constructed on the basis of thermally activated screw dislocation glide. We apply the methodology to yielding in tungsten and show that available experimental measurements can be explained and reproduced by accounting for these two very important features of BCC plasticity. The validated methodology is used to predict strength as a function of several state variables in W single crystals.

(G10 invited) **Elasto-plastic behaviour of nanostructured bcc iron columnar structures**

J G Sevillano[1], J Aldazabal[1], I Aldazabal[2] and A Luque[3]

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We explore, using molecular dynamics (MD), the potential strength and mechanical stability at 300 K of pure bcc Fe with a strongly oriented columnar structure of <011> grains of average size ranging from 20 to 5 nm in the cross-section. According to the simulations, their tensile flow stress would span from 4 to 6 GPa. The structure of axially oriented tilt boundaries is very stable to plastic elongations as large as 50%.

The obvious connection of this exercise is with fine wires obtained by drawing high melting point bcc metals or alloys that reach record mechanical strength because of the extraordinary strain hardening associated to their <011> wire texture concomitant with the development of a columnar structure of axially oriented grains of nanometric cross section. For Fe-0.007%C drawn to a true strain of 10 (conventional wire drawing is technologically limited to such strain), the grain size evolves from tens of microns to about 100 nm, the tensile strength reaches 2 GPa and the strain hardening does not display any sign of being exhausted.

(G10 oral) **Heterogeneous deformation in ductile FCC single crystals in biaxial stretching: the influence of slip system interactions**

J-L Dequiedt, C Denoual, R Madec

CEA, DAM, DIF, France

The deformation of ductile single crystals often evolves from an initial homogeneous deformation to a strongly heterogeneous one. In some cases, this is triggered by the propensity of slip systems to segregate in order to minimize their mutual interactions. In this work (also published in JMPS (2015), 83, 301-318) the phenomenon is investigated by both crystal plasticity simulations and an analytic approach in FCC's crystals in biaxial stretching, for which a large number of systems is involved. The constitutive behaviour is based on a generalized storage recovery model, previously calibrated by dislocation dynamics, in order to take precisely into account the interactions between slip systems. The simulations demonstrate the key role of the interaction matrix and display a partition of slip systems driven by the strongest interaction, in general the collinear interaction between cross-slip systems. The lamellar-type of obtained microstructure can be justified theoretically as a band-type instability mode of the homogeneous deformation of the crystal. This analysis also gives a simple way to evaluate the sensitivity of the partition process to the relative strength of the different interactions. A comparison with an experimental study in simple shear yields useful information about some of the terms of the interaction matrix.

(G10 oral) **Multiscale investigation of strain aging phenomena of pure alpha titanium**

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Strain aging phenomenon has been recognized as one of the major cause of unusual viscoplastic behavior of titanium observed at room temperature. Particularly the phenomena of static and dynamic strain aging have been the object of multiple researches lately. To date the issue of strain aging in Ti and its alloys stays debatable and needs a further investigation.

The experimental studies on commercially pure alpha Ti revealed a yield stress anomaly corresponding to static aging peak when the material is loaded in transverse direction. The origin of the anomalous yield point can be attributed to the interaction of the activated <c+a> dislocations with interstitial atoms of oxygen resulting in pinning-unpinning process conforming Cottrell aging. Portevin- Le Chatelier effect observed at the lower strain rates was ascribed to the non-planar core of screw <a>-type dislocations.

Based on the proposed scenario, a new phenomenological elastic-viscoplastic strain aging model coupled with crystal plasticity is formulated to simulate the static and dynamic strain aging effects. This approach allows to take into account the local arrangement of grains and detailed description of their slip systems necessary to understand the heterogeneity in strain field space and time distribution. An additional variable t_a called aging time was introduced to simulate the age hardening phenomena. Finite element simulations are performed on polycrystalline aggregates with various numbers of grains accounting for the elastic and plastic anisotropy of alpha-Ti. Depending on the set of chosen parameters the model can be used for both static and dynamic strain aging simulations.

(G10 oral) **Atomistically-informed crystal plasticity in MgO polycrystals under pressure**

J Amodeo[1], S Dancette[1] and L Delannay[2]

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This study addresses multi-scale modeling of a special kind of pressure-dependent plasticity. In MgO, which is a major constituent of the Earth's lower mantle, the relative activity of the 1/2⟨110⟩{110} and 1/2⟨110⟩{100} slip modes depends on the level of hydrostatic pressure. The influence of pressure on both the dislocation core structures and the collective behavior of dislocations may be computed based on atomistic modeling and dislocation dynamics simulations. In the present study, results from such lower-scale simulations are used to determine the parameters of a crystal plasticity model that is suitable in order to probe the large-scale mechanical response of MgO polycrystals at pressures up to 100 GPa. The model is assessed based on experimental compression tests performed at different pressure levels. It turns out that the responses of single crystals and polycrystals are fundamentally different. Moreover, due to the large anisotropy of individual crystals, the outcome of polycrystalline simulations is found to depend strongly on the modeling assumption made about grain interactions. Crystal plasticity based finite element modeling provides the best predictions of the texture development when comparing to recent high pressure experiments.

(G10 oral) **Dislocation based modelling for nuclear ceramics viscoplastic behaviour**

L Portelette and B Michel

CEA, France

This paper focuses on the numerical simulation of mechanical behaviour at microscopic scale in nuclear fuel ceramics. The purpose of this study is to model viscoplastic behaviour of polycrystalline uranium dioxide using a dislocation based approach. Constitutive equations of the model for UO2 single crystal behaviour are determined according to the experimental results of Sawbridge. In the latter active glide systems are characterized as a function of the crystal orientation in a compressive test at high temperature (1660 K). Due to crystallographic fluorite structure of UO2 gliding systems are quite complex to analyse, and cannot be only deduced from the Schmid factor computation for gliding planes with the highest atomic density. According experimental works it has been shown that there are three families of gliding systems involving dislocations respectively characterized by planes {100}, {110} and {111}. In previous studies a first formulation of the dislocation based model has been proposed in order to explain the viscoplastic anisotropy of UO2. In this study an improvement of the dislocation based model is proposed in order to have a better description of the macroscopic yield stress as a function of the crystal orientation. This improvement is possible through the third gliding systems family in order to avoid locking strain mechanisms due to the geometrical characteristics of the first gliding system family. After this, some finite element simulations of the viscoplastic behaviour at the polycrystalline scale will be presented in order to quantify the impact of the single crystal anisotropy on microscopic stress-strain field.

(G11 invited) **Time evolution of the velocity distribution of dislocations**

I Groma and P Ispánovity

Eötvös University, Hungary

Determining the properties of the velocity distribution of dislocations is of key importance for understanding the physical origin of the phenomenological continuum theories of dislocations.

In the first part of the presentation some analytical properties of the probability distribution of the velocity of dislocations are discussed. It is shown that the distribution has an inverse cubic tail. The theoretical result is verified by discrete dislocation dynamics simulations and experimental results on 2D crystals.

In the second part the time evolution of the velocity distributions obtained by 2D and 3D discrete dislocation dynamics simulations are analysed during the relaxation of an initially random dislocation system [1] and under monotonic loading [2]. It is demonstrated that the velocity distribution exhibits power law type of scaling properties with a cut of depending on the system size.

Financial supports of the Hungarian Scientific Research Fund (OTKA) under contract numbers K 105335 and PD105256 and of the European Commission under grant agreement No. CIG 321842 are acknowledged.

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(G11 oral) **Mesoscale theory of dislocations: from the discrete to the continuum**

A Finel, P-L Valdenaire, Y LE BOUAR and B Appolaire

LEM (ONERA/CNRS), France

Plastic deformation of crystals involves the motion and interaction of discrete dislocations. However, because of the enormous range of time and space scales involved in dislocation dynamics, plastic modeling at macroscale requires a continuous formulation.

In this talk, we present a rigorous formulation of the transition between the discrete, where plastic flow is resolved at the scale of individual dislocations, and the continuum, where dislocations are represented by densities.

First, we focus on the underlying coarse-graining procedure and show that the emerging correlation-induced stresses are scale-dependent. We also show that these local stresses contains symmetry-breaking components that make the stress experienced by dislocations to depend on the sign of their Burgers vector. We also show that, on top of the gradient of the geometrically necessary dislocation density, the emerging back stress contains a component that depends on the gradient of the total dislocation density.

Finally, we show that these correlation-induced stresses may generate dislocation patterning even in the simplest situation where parallel dislocations are allowed to glide along a single slip system.

(G11 oral) **The role of weakest links and system size scaling in multiscale modelling of stochastic plasticity**

P D Ispánovity, D Tüzes, P Szabó and I Groma

Eötvös University, Hungary

Plastic deformation of crystalline matter often involves intermittent local strain burst events. To model this phenomenon on the mesoscale stochastic plasticity models were introduced, where microstructural details are represented by a fluctuating local yielding threshold. Although these models proved successful in recovering several experimentally observed features (for instance, scale-free distribution of strain burst sizes) not much effort has been made to understand the role of the parameters of the models, like the distribution of the local yielding threshold.

In the present talk we present numerical results on lower-scale discrete dislocation dynamics (DDD) simulations and the stochastic crystal plasticity model (SCPM) in terms of statistical properties of the fluctuating stress-strain curves. We demonstrate that the results can be explained by a theoretical plasticity model based on the subsequent activation of the weakest spots in the material. The theory lets us identify the key exponents characterizing, e.g., the local yielding threshold distribution or the system size dependence of the typical strain burst sizes. Multiscale modelling is achieved by determining these exponents for the DDD models and inserting them into the SCPM. The success of scale-linking is demonstrated by the statistical analysis of the stress-strain curves obtained by the resulting mesoscopic and the discrete dislocation models of various system sizes.

In the end of the talk we discuss connections between recent 3D DDD simulations, micropillar compression experiments and the present results. We also highlight that the proposed technique of multiscale modelling is expected to be applicable for different microstructures and amorphous materials, too.

(G11 oral) **Investigation of creep and load shedding in polycrystalline titanium alloys using discrete dislocation plasticity**

Z Zheng, D Balint and F Dunne

Imperial College London, UK

Titanium alloys have been used for highly stressed components in military and commercial aircraft engines for over 60 years. Dwell sensitivity is well known in alpha-Ti or near-alpha alloys, which is associated with high stresses at grain boundaries caused by dislocation pile-ups that can initiate facet fracture. The mechanism of dwell debit, quantified as the reduction in fatigue life when the cyclic loading includes a hold at the peak stress, is thought to be related to very particular crystallographic orientation combinations. A polycrystalline aggregate containing a combination of a primary hard grain with c-axis nearly parallel to the loading direction and adjacent soft grains with c-axis nearly normal to the loading direction, commonly known as a rogue grain combination, was studied under a dwell fatigue condition using a discrete dislocation plasticity model. A thermal activation process for dislocation escape from obstacles was incorporated in order to account for the observed rate sensitivity of this material at low strain rates. The activation energy of the obstacle escape process was determined for Ti6242 and Ti6246 by fitting a consistent crystal plasticity model to experimental data. Load shedding was found to occur within the rogue grain combination, in which stress is redistributed from the soft grain to the hard grain during a hold at peak applied stress, but only in Ti6242 despite a relatively small difference in the activation energies found for these alloys. This appears to explain the experimental observation that Ti6242 experiences significant dwell debit, whereas Ti6246 does not.

(P1.37) **Modeling plasticity of MgO at the mesoscale by 2.5D Dislocation Dynamics**

R Reali, F Boioli, P Carrez, K Gouriet and P Cordier

Université Lille 1, France

(Mg,Fe)O ferropericlase is a major constituent of the Earth's lower mantle. Understanding how this phase deforms is thus of primary importance in geophysics.

Since dislocation motion is one of the most efficient strain producing mechanisms, in this study, we investigate the contribution of dislocations to the plastic deformation of MgO at the mesoscale, by using Dislocation Dynamics (DD) simulations. In particular, we rely on the so-called 2.5D DD approach, where dislocations are considered as straight segments perpendicular to a 2D reference plane and local rules are applied to mimic the 3D behavior. In this framework, both the glide and climb mechanisms can be taken into account.

In order to address the deformation of MgO under pressure, temperature and strain rate conditions expected in the lower mantle, we first benchmark our model at ambient pressure, by comparing our simulation results with experiments and other numerical simulations performed in the same conditions.

Deformation of MgO is investigated at low (100-450 K), intermediate (1000 K) and high temperatures (1500-1800 K), in order to characterize the different strain-controlling mechanisms which are dominant in these three regimes.

Results are found in agreement with previous experimental and numerical data, confirming that the underlying physical processes are well described and allowing to further investigate the plasticity of MgO at lower mantle conditions.

(P1.38) **The role of dislocation pile-up in flow stress determination and strain hardening**

K Schulz[1], Y Zhu[2] and P Gumbsch[1]

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The striving for advanced materials with well-defined microstructures has also led to an increasing effort towards a physically based description of the motion of dislocations as the cause of plastic deformation and the origin of materials failure. Several dislocation based continuum theories have been introduced, but only recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor.

Regarding a self-consistent coarsening of dislocation modelling in order to construct an efficient numerical implementation, several issues have to be solved including calculation of the stress field of a system of dislocations, correlation functions, and boundary conditions. Accurate solutions have already been found for single slip systems.

In this presentation, the widely used Taylor-type hardening relation is discussed for glide plane intersections. In the context of a continuum model, we introduce formulae which resolve more details from the underlying discrete dislocation dynamics. Here, the shear flow stress is found weaker than the critical resolved shear stress to remobilise a singly locked primary dislocation, because dislocations can dynamically pile up against junctions resulting from dislocation interactions. Considering the derived formulae, the roles played by dislocations belonging to different slip systems in strain hardening are further discussed.

(P1.39) **Meso-scale simulation of dislocations in irradiated uranium dioxide using two-dimensional dislocation dynamics**

A Lunev

Joint Institute for High Temperatures of the Russian Academy of Sciences, Russia

In nuclear fuel based on uranium dioxide (UO_2) irradiation generates a large density of dislocations. Hence, the evolution of microstructure under irradiation may happen due to plastic flow. However, very little is known yet about the accumulation and interaction of dislocations in oxide nuclear fuel. So far, the properties of dislocations in UO_2 were studied mostly by molecular dynamics. Rate theory was also applied to describe the long-term accumulation of dislocations. However, using these methods it is impossible to model tangled dislocation networks observed in high burn-up fuel. At the same time, a consistent experimental study requires representative sampling, which in case of in-pile tests could hardly be achieved. This presentation will deliver the results of on-going work on meso-scale computer simulation of dislocation structures in oxide nuclear fuel using two-dimensional dislocation dynamics. In addition, a brief summary of experimental studies of dislocations in ion-irradiated UO_2 (X-ray diffraction, atomic-force microscopy) performed earlier by the author will be reported.

(P1.40) **Multiscale theory for the climb of jogged dislocations**

P-A Geslin[1], B Appolaire[2] and A Finel[2]

[1]Université Lyon 1-CNRS, France, [2]Laboratoire d'Etude des Microstructures, Onera/CNRS, France

At elevated temperature, dislocations change glide planes by absorbing/emitting vacancies. This climb process allows different precipitates bypass mechanisms and influences significantly the creep response of metals and alloys. In face-centered cubic metals and alloys, vacancies are absorbed on specific defects, called jogs, along the dislocation. Due to their high energy, the density of these defects can be low. In previous approaches, the influence of the low jog density is generally ignored or at best treated approximately. In this work, we first propose an analytical solution for the climb rate of a jogged dislocation that accounts for fast pipe diffusion in the dislocation core and for the energy barrier for the jump of a vacancy between the dislocation core and the bulk. In a multiscale approach, we then present a mesoscale phase-field model for dislocation climb that accounts for transient climb regimes and for the complexity of the diffusion field around an ensemble of dislocations. An asymptotic analysis of the model allow to link quantitatively the dislocation climb rate to the parameters of the model. In particular, the kinetic parameter of the phase-field can be chosen to reproduce quantitatively the climb rate of dislocations with a low density of jogs.

(P1.41) **Investigation of the strengthening induced by coherent precipitates with dislocation dynamics**

S Queyreau[1], S Aubry[2], E Tarleton[3] and T Arsenlis[2]

[1]LSPM CNRS - Univ. Paris XIII, France, [2]Lawrence Livermore National Laboratory, USA, [3]University of Oxford, UK

In precipitation-hardened alloys, dislocations have the possibility to shear coherent second phase particles that exhibit the same crystallographic structure as the main phase. The detail of the interaction between dislocations and shearable particles is comparatively less understood than in the case of impenetrable incoherent particles and is associated to various atomistic mechanisms suggested in the literature. In this study, we propose a coupling between Dislocation Dynamics and Finite Element Method that accounts for different mechanisms observed in atomic simulations. (i) The dislocation shearing generates a surface step at the void surface that is associated to an increase of potential energy. (ii) A part of the dislocation line (and core) energy is different inside a particle. And (iii) the distant interaction induced by the elastic stress fields of the dislocation and precipitates. The evaluation of tractions induced by dislocation microstructures on the particle surface is performed analytically and using non-singular continuum theory of dislocations. We illustrate this modelling of dislocation-particle interaction in the case of several particle types introduced in a bcc iron matrix.

(P1.42) **Hydrogen and helium solute effects on screw dislocations in bcc Fe and W from first principles**

L Ventelon and F Willaime

CEA, France

Using Density Functional Theory (DFT), the interaction between the screw dislocation core and hydrogen/helium solutes is calculated in body-centered cubic (bcc) Fe and W at different solute concentrations along the dislocation line. As in the case of carbon solutes in bcc metals [1], we demonstrate that hydrogen and helium solutes destabilize the usual easy core to the benefit of the hard core configuration of the screw dislocation, which is unstable in pure bcc metals. H and He solutes are at the center of a regular prism in a cementite like local environment. Considering the crystal zero-point vibrations, attractive H and He-screw dislocation interaction energies ranging from -0.6 to -0.3 eV were found in both Fe and W for interstitial sites within the dislocation core. This unexpected low-energy configuration leads to dislocation core saturation by solute atoms, even for very low bulk solute concentrations. This core reconstruction will constitute an essential factor to take into account in irradiation-induced phenomena, such as hydrogen embrittlement and void swelling.

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(P1.43) **The Bauschinger effect in highly confined thin films: a discrete dislocation plasticity study**

S Waheed, R Hui, D Balint and F Giuliani

Imperial College London, UK

Understanding the mechanism of plasticity in confined thin films is crucial to the reliable functioning of nano/micro electromechanical machines (NEMS/MEMS). In this study, sequential sputter deposition, diffusion bonding and focused ion beam milling are used to fabricate Sapphire micropillars encapsulating a thin single crystal Niobium film. A distinct Bauschinger effect is observed during the cyclic axial compression of the samples. Plain strain discrete dislocation plasticity (DDP) is used to interpret the experimental results obtained for the encapsulated film-micropillar geometry and the O'Day method [1] implemented to model the elastically heterogeneous specimen. The simulations show that the experimental samples correspond to a saturated source density regime, producing the maximum Bauschinger effect for the chosen mean nucleation strength. This is attributed to the large amount of junction formation that would occur in a highly confined small volume. Next, the source density and mean nucleation strength are shown to have a coupled effect on the size of the Bauschinger effect. This is understood in terms of the differing number of pile-ups occurring per source in the film and, hence, the number of dislocations available for reverse glide. The coupled effect is found to be represented by the density of dislocations annihilated upon unloading: a consistent linear relationship is observed between the size of the Bauschinger effect and the annihilated dislocation density over the entire parameter space investigated.

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(P2.20) **Atomic scale insights on the microstructure evolution of urania under irradiation**

A Chartier and L Van Brutzel

CEA-Saclay, France

Urania is commonly used as a fuel in nuclear industry. Urania is heavily irradiated during its in-reactor stay, and faces drastic microstructural modifications, including few percent's swelling and increase of dislocation density. Dislocations are identified as perfect dislocations loops which transform with increasing fluence into lines at sufficiently high temperature – i.e. at 600 °C. However, the early stages of their nucleation are hardly attainable experimentally. One commonly infers that their nucleation is related to the aggregation of point defects or defects clusters into dislocations.

In the present paper, we clarify the first steps of the effect of irradiation on urania by means of molecular dynamics simulations using empirical potentials. The irradiation dose is simulated by continuous accumulation of Frenkel pairs at 600°C, skipping the cpu-expensive displacement cascades.

Starting from a defectless urania, we observe the nucleation and growth of dislocations under Frenkel pairs accumulation. Detailed analysis shows a four stages evolution : (i) an increase of point defects (ii) then the nucleation of Frank loops 1/3 <111> from the aggregation of point defects, (ii) the transformation of Frank loops into perfect loops 1/2 <110> (iv) and finally their stabilization as lines. Our simulations also show a swelling up to 3.2% during the first stage in which point defects are present. This swelling suddenly decreases to 1.5% in the second stage, as soon as dislocations nucleate.

Both stage (iv) and swelling agree with experimental data and therefore strengthen the four stages scenario of the microstructure evolution of urania under irradiation.

(P2.21) **Narrow dislocation dipoles in deformed intermetallic gamma-TiAl**

H Wang[1], G Zhou[1], D Xu[1], R Yang[1] and D Rodney[2]

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Dislocation dipoles play important roles in the plastic deformation of materials. For instance, the formation of a stable dipole locks the two constituent dislocations and contributes to work hardening; dipole annihilation after dragging a jogged screw dislocation produces vacancy- or interstitial-type defects, which contribute to deformation localization; etc. In intermetallic g-TiAl, dislocation dipoles in the form of faulted dipoles are frequently encountered in deformed samples [1], but their fine structure and transformation into point defects remain largely undocumented. In the present work, narrow dipoles in g-TiAl with height lower than 6*d* (with *d* the {111} interplane spacing) are systematically investigated using atomistic simulations. The stability of narrow dipolar configurations are unraveled by interatomic potential and *ab initio* calculations, showing the stability of faulted dipoles over other forms. The results are compared with transmission electron microscopy observations [2]. Subsequent direct molecular dynamics simulations indicate that at elevated temperature, these dipoles transform into individual defects, e.g., vacancy clusters, stacking fault tetrahedra and interstitial loops, depending on dipole height and orientation. Employing saddle-point search methods, activation energies of the atomic processes therein are obtained and the lifetime of the deformation debris is estimated, showing the stability of certain narrow dipoles on the experimental timescale. Lastly, the influence of stable narrow dipoles on plastic deformation is discussed.

Dr. Patrick Veyssière (1947-2011) initiated and contributed to the research.

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(P2.22) **On effective mobility of BCC dislocations in two-dimensional discrete dislocation plasticity**

T Katiyar and E van der Giessen

University of Groningen, Netherlands

Within a multiscale program on the physics of failure, we aim to establish a micromechanical understanding of the interfacial decohesion between a hard particle and a body-centered cubic (BCC) matrix at the size scale of micrometers. This will be done using two-dimensional discrete dislocation plasticity (2D-DDP) in conjunction with cohesive surfaces. The existing 2D-DDP framework has been applied to fracture problems but, so far, is limited to FCC materials. One of the key challenges in extending the method to BCC materials is that, contrary to FCC, the mobilities of edge and screw dislocation segments are vastly different from each other in BCC materials. We here propose to map the edge and screw mobilities of 3D dislocation loops into an effective mobility of edge dislocations in 2D. In this poster, two approaches of the basic idea to equate plastic slips in 2D and 3D are presented. We report 2D-DDP simulations to validate the predictions of rate sensitivity in Iron polycrystals against experimental values.

Symposium H

(H1 invited) **Direct HRTEM observation of the clustering process of self-interstitial atoms in iron**

K Arakawa[1], S Arai[2], C Marinica[3], E Meslin[3], F Willaime[3], T Amino[4], P Olsson[5], S Dudarev[6], Y Zhang[7], Y Oshima[8] and N Tanaka[2]

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Ferritic steels are key materials for nuclear-fission and fusion reactors; therefore, the full understanding of the radiation-damage processes within them is strongly required. However, even clustering process of radiation-produced self-interstitial atoms (SIAs) in iron has not been fully uncovered. In a long-standing well-accepted model, <110> dumbbell SIAs cluster to form prismatic imperfect dislocation loops with the Burgers vector of 1/2<110>, as the precursors of nanoscale 1/2<111> and <100> perfect dislocation loops [1]. In contrast, in a recent revolutionary model, it has been proposed that small SIA clusters can have the C15-Laves structure [2]. However, there have been no experimental evidence for the existence of either 1/2<110> dislocation loops or C15 phases.

In this presentation, we will show our recent results of the first successful direct high-resolution transmission electron microscopy observation of the clustering process of SIAs in iron. We observed the frequent formation of the small C15-like phases upon high-energy electron irradiation, within a high-voltage electron microscope. Some of C15-like phases were annihilated under irradiation. On the other hand, comparatively large C15-like phases growing into approximately 2 nm in diameter transformed into 1/2<111> dislocation loops.

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(H1 oral) **Effect of irradiation on chromium precipitation in ferritic steels**

F Soisson

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Iron-Chromium alloys are the model system of ferritic alloys that will be used in future fusion or fission nuclear reactors. During isothermal annealing of Fe-Cr alloys, one may observe equilibrium segregations on extended defects (e.g. Cr enrichments at grain boundaries) and the coherent precipitation of the Cr-rich α' phase in supersaturated alloys (e.g. above 15at.% Cr at 500°C). Several experimental studies have shown that irradiation can considerably affect these behaviors, and therefore the corrosion resistance and mechanical properties of ferritic alloys. Specifically, irradiation may lead to (i) a radiation-induced segregation that can reinforce or oppose equilibrium segregation, (ii) the acceleration of α' precipitation in super-saturated alloys, and (ii) a radiation-induced α' precipitation in under-saturated alloys.

We present Atomistic Kinetic Monte Carlo simulations that can model these different phenomena within a common framework, using a diffusion model including vacancy and self-interstitial mechanisms. The Monte Carlo parameters are fitted on ab initio calculations.

The results of the simulations are compared with available experimental studies, especially recent observations of accelerated precipitation under neutron, ion and electron irradiations. The effects of alloy composition, temperature and dose rate are considered.

(H1 oral) **Numerical and experimental determination of the formation and properties of nanometric-sized helium-filled bubbles in semiconductors**

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Cavities (filled or not) are a major type of extended defects usually resulting from the incorporation of inert gas or hydrogen in solids by high fluence implantation or transmutation reactions. While these defects are of major interest in several domains, from materials for microelectronics and energy, to more fundamental fields (study of plasmon excitations or nanofluidics), our understanding of the mechanisms of formation and evolution under thermal annealing remains severely limited. To improve the current state of the art, we applied a multiscale methodology combining first-principles calculations, molecular dynamics simulations, and quantitative TEM analysis. We focused on helium-filled bubbles in silicon and silicon carbide. Starting from a single impurity in interaction with intrinsic defects, the first steps of bubbles formation were determined. Dedicated interatomic potentials were then fitted with these results, and used to perform large scale molecular dynamics simulations of bubbles with diameters from 1 nm to 7 nm. These simulations allowed for the determination of the helium density and the internal pressure in these bubbles, the former quantity being compared to experimental measurements made on bubbles of similar sizes with STEM-EELS and a newly developed energy-filtered TEM spectrum imaging procedure. Finally, by varying the temperature and the bubble internal pressure, we determined the phase transition of helium, as well as the plastic deformation of the surrounding matrix.

(H1 oral) **Artificial Neural Network based cohesive model from ab initio: principles and applications to single point-defect migration in binary Fe-based alloys.**

N Castin[1], L Messina[2], C Domain[3], R C Pasianot[4] and P Olsson[5]

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In recent works [1-2], we have proposed an innovative approach to KMC simulations in which transitions rates are predicted by an artificial neural network (ANN) trained on migration barriers obtained with density functional theory (DFT). Novelty compared to previous approaches also based on ANN trained from interatomic potentials [3] resides in a systematic reference to DFT, thereby avoiding approximations in the fundamental physics of the studied alloy.

In this work, we present a continuation of the approach by reinforcing the use of DFT in KMC models. The transition-state model is first reformulated to decompose the contribution to kinetics from end-states energies and from the relative height of the saddle-point during transitions. Next, dedicated ANN's are used to play the role of rigid-lattice cohesive models directly fitted from DFT energies, thereby providing strong bases for the accurate description of equilibrium states. Finally, the same approach is naturally extended for the definition and fitting of lattice-free ANN interatomic potentials, providing efficient numerical methods for estimating migration energies as obtained from DFT.

The methodologies and principles are demonstrated on FeCu and FeCr alloys, considering the migration of either kind of point-defects (vacancies and self-interstials).

[1] L. Messina, N. Castin, C. Domain, and P. Olsson, "Introducing ab initio-based neural networks for transition-rate prediction in kinetic Monte Carlo simulations", submitted for publication
[2] L. Messina, N. Castin, C. Domain, and P. Olsson, MM2016 conference, this book of abstracts
[3] N. Castin, M. I. Pascuet, and L. Malerba, The Journal of chemical physics 135, 064502 (2011)

(H1 oral) **Modeling the pressure vessel steel microstructure evolution under neutron irradiation - input from ab initio calculations in Fe multi component alloys**

C Domain[1], B Pannier[1] and C Becquart[2]

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The ageing and the evolution of mechanical properties of pressure vessel steels under radiation has been correlated with the formation of more or less dilute solute clusters. In the dilute Fe alloys, tomographic atom probe analysis show that these clusters are mainly enriched in Cu, Ni, Mn, Si, P. The evolution of these features is governed by the migration of the individual point defects. Understanding the mechanisms responsible requires the use of atomistic simulation to obtain insights on the diffusion and agglomeration of both point defects and solute atoms. Density Functional Theory calculation results on the interaction of substitutional solutes and carbon with different extended defects (small vacancy and solute clusters, as well as interstitial loops) will be examined, and their use to improve the energetic model of kinetic Monte Carlo will be presented. In particular we will discuss their impact on the evolution of the microstructure under irradiation modelled by Atomic Kinetic Monte Carlo.

(H2 invited) **Impurity flux coupling and anomalous swelling in iron**

P Olsson[1], L Messina[1], Z Chang[1], M Nastar[2], N Sandberg[3], D Terentyev[4] and K Samuelsson[1]

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Irradiation driven diffusion in metals can lead to many phenomena with macroscopic implications. Radiation induced segregation, driven by flux coupling, and irradiation induced swelling are two such examples.

Electronic structure theory was used here as the physics basis for a systematic self-consistent mean field study of impurity diffusion and flux coupling in dilute iron alloys, with impurities from the full transition metal series as well as Al, Si and P. The d-band filling is shown to govern most properties for the transition metal impurities except for the strongly magnetic ones. Predictions of diffusivities are given from low to high temperatures including the a treatment of the effects of the magnetic phase transition in iron. The mechanisms for slow diffusion is well understood and Co, Re, Os and Ir are such impurities. Vacancy drag is confirmed as the dominant flux coupling mechanism at low temperatures with few exceptions.

Swelling is a complicated phenomenon with several acting driving forces but the dislocation bias is included in all current models. Here, atomistic calculations of defect-dislocation interactions are coupled with anisotropic elasticity and a finite element solver for the steady state defect diffusion. Capture efficiencies and dislocation bias is obtained for edge and screw dislocations in fcc nickel and bcc iron. Anomalous capture tendencies are show for both dislocations in iron. Most importantly, a negative bias is predicted for the screw dislocation, which gives rise to a new mechanism for the high incubation dose for steady state swelling seen in iron and iron alloys.

(H2 oral) **Scaling laws for formation energy of large interstitial clusters in V, W and Fe from ab-intio simulations**

R Alexander[1], M-C Marinica[2], L Proville[2], F Willaime[2], M R Gilbert[3] and S L Dudarev[3]

[1]CEA, DEN, Service de Recherches de Metallurgie Physique, France, [2]CEA, DEN, Service de Recherches de Metallurgie Physique, France, [3]EURATOM/CCFE Fusion Association, Culham Centre for Fusion Energy, UK

Study of defects in the body centered cubic crystals serves as the basic foundation for future research regarding structural materials and pave the way for a better understanding of materials aging. The dislocation loops at nanometric size are too small to be characterized by the experiment or too big to be investigated by a reliable energetic model as ab-initio. In this presentation we propose the development of an energetic model for the self-interstitial clusters in body centered cubic metals which is able to predict the relative stability of large self-interstitials clusters up to nanometric-size directly from ab initio calculations performed on small clusters. We will apply this model in the case of Fe, W and V. We will give particular attention to the relative stability of the traditional dislocation loops with and ½ orientations as well as the C15 clusters. Those C15 clusters form three dimensional structure which the symmetry corresponds to C15 Laves phase embedded in body centered cubic matrix [2]. The theoretical findings of the new energetic model will be compared with recent experiments. The implication of the relative stability of C15 clusters against planar loops will be discussed in the framework of the proposed mechanism of the transformation of C15 clusters into or 1/2 loops [2].

[1] M.-C. Marinica et al. Phys. Rev. Lett., 108, n025501, (2012)
[2] Y. Zhang et al. Scripta Mat. 98, 5 (2015)

(H2 oral) **DFT study on the contribution of phonon and electron excitations to the free energy of embedded defect clusters**

M Posselt and D Murali

Helmholtz-Zentrum Dresden-Rossendorf, Germany

Modeling of nanostructure evolution in solids requires the knowledge of comprehensive data on the properties of point defects and defect clusters. Since most processes occur at elevated temperatures not only the energetics of the defects in the ground state but also their temperature-dependent free energy must be known. The determination of the contribution of phonon and electron excitations to the free binding energy of small embedded defect clusters is illustrated in the case of bcc-Fe. The fundamentals of the first-principles calculation method have been recently described [1]. First of all, the ground state properties of the clusters are determined under zero pressure (ZP) conditions. Second, the phonon contribution to the free energy is calculated within the harmonic approximation using the equilibrium atomic positions determined in the ground state. The application of a quasi-harmonic correction to the ZP-based data does not modify the results significantly. Therefore the obtained data are valid under zero-pressure conditions at higher temperatures than in the framework of the purely harmonic approach. These conditions are usually realized in experiments. Third, the contribution of electron excitations to the defect free energy is calculated. The electron excitations can lead to an additional deviation of the total free energy from the ground state value or can compensate the deviation caused by the phonon contribution. Depending on the examples considered the free binding energy of a defect cluster can differ significantly from the ground state value.

[1] D. Murali, M. Posselt, M. Schiwarth, Phys. Rev. B 92, 064103 (2015)

(H2 oral) **Anomalous vacancy-assisted chromium segregation in FeCr alloys**

M Lavrentiev, D Nguyen-Manh and S Dudarev

Culham Centre for Fusion Energy, UK

Recent experimental observations show the formation of chromium clusters in ion-irradiated dilute FeCr alloys in the Cr concentration range well below the 10 at.% threshold, above which the alloys exhibit Cr segregation. The origin of this anomaly remains unclear, however the fact that it occurs under irradiation suggests that vacancies and small vacancy clusters might act as catalysts, facilitating Cr segregation, in this way changing the kinetics of alloy decomposition under high temperature and high irradiation dose conditions. We have investigated the possible occurrence of chromium segregation near vacancies in dilute Fe-Cr alloys using ab initio calculations. We find that vacancies can serve as nucleation centres for chromium atoms, attracting up to five Cr atoms to a monovacancy. For the latter case, the most stable configurations correspond to Cr atoms arranged as third nearest neighbours. For these configurations, the binding energy per Cr atom is close to 0.1 eV, with the energy of a 4Cr-1Vac cluster being $\sim$ 0.4 eV lower than the energy of a random configuration. Configurations involving second nearest neighbour Cr atoms are energetically unfavourable and have negative binding energies, starting with four Cr atoms around a vacancy. A linear fit to the numbers of second, third and fifth nearest neighbours describes the binding energy of Cr-vac clusters very well. Absolute values of magnetic moments of Cr atoms in the energetically favourable configurations are substantially larger than in the unfavourable configurations, highlighting the magnetic nature of the anomalous Cr-vacancy segregation effect.

(H3 invited) **MMM and the challenge of driven materials**

G Martin

The discovery, 50 years ago, of irradiation induced swelling of steels in fast breeder reactors, stimulated a large amount of experimental work, in particular on model materials irradiated by neutrons or charged particles, as well as several theoretical developments, new modeling techniques and atomistic simulations.

Indeed, not only irradiation, but also sustained plastic shearing, friction, etc. do drive materials away from their equilibrium state, at best toward some stationary dynamical state(s). The kinetic pathway of such evolutions, and as a result the time evolution of materials properties, as well as the stability of the stationary state(s) eventually reached, still lack as versatile a theoretical framework, as is thermodynamics for equilibrium states.

A brief survey of the state of the art and of open challenges will be given for phase stability in driven multicomponent alloys.

(H3 oral) **Segregation and precipitation on defect clusters: A phase field approach**

P Bellon, T Garnier, D Trinkle and R Averback

University of Illinois, USA

Segragation and precipitation under irradiation in alloys is a well known phenomenon, driven by the coupling between chemical and net defect fluxes to sinks such as surfaces, grain boundaries, and dislocations. Nanoscale characterization often reveals the formation under irradiation of solute clusters. Some of these clusters are not associated to dislocation loops or lines, so they cannot have simply formed by radiation-induced segregation on defect sinks. Irradiation-induced homogeneous precipitation is a possible mechanism, but linear stability analysis of diffusion models has shown that the conditions for this instability are quite restrictive. We propose here an alternative mechanism, whereby exhaustible sinks, such as small interstitial and vacancy clusters created in displacement cascades, promote the dynamical stabilization of chemical clusters, even in undersaturated solid solutions. Using phase field modeling, we demonstrate on model alloys that this mechanism is very effective, even when the coupling between point defects and solute is not sufficient to trigger an instability by Frenkel pairs only. The relevance to Ni-base and Fe-base alloys is discussed.

(H3 oral) **Coupling radiation damage from binary collision Monte Carlo to phase field microstructure evolution**

D Schwen, Y Zhang and S Schunert

Idaho National Laboratory, USA

Nuclear fuels and reactor-core components experience a significant amount of particle irradiation during their operational lifetime. The accumulating radiation damage has a strong influence on the material properties both directly and indirectly by impacting the microstructural evolution, which in turn modifies the neutron transport characteristics of the material.

Based on INL's Multiphysics Object-Oriented Simulation Environment (MOOSE) framework, a damage production model has been developed that can use either empirical primary knock on atom (PKA) mass and energy distribustions as well as PKA populations informed by neutron reaction data obtained through a concurrent neutron transport simulation to perform cascade simulations on samples of ongoing phase field microstructure evolution simulations. The PKA energy and mass distributions are a function of the sample microstructure and thus spatially varying. Cascade simulations are performed using a binary collision Monte Carlo code and the defect fields are communicated back to the finite element based phase field simulation where they are used as a source terms in the microstructure simulation component.

We demonstrate this capability on heterogeneous microstructures such as surrogate systems of oxide dispersed steels under irradiation.

(H3 oral) **Design of radiation-resistant alloys**

T Schuler, D Trinkle and P Bellon

MatSE, University of Illinois Urbana-Champaign, USA

The design of nanoscale microstructure is a promising way to develop radiation-resistant alloys. These microstructures can be obtained under out-of-equilibrium processing routes. The main issue with such materials is to ensure the stability of the microstructure under high fluxes and/or at high temperatures.

In our attempt to develop such materials, we combine various techniques to study the thermodynamic and kinetic properties of copper alloys, in which some solutes are added. The goal is to obtain a fine and homogeneous distribution of these solutes, or solute-defect clusters, in order to pin dislocations. Starting from the electronic scale, we obtain binding energies and migration energies of point-defects and solutes in various local chemical environment. Then, we apply the self-consistent mean-field formalism to compute transport coefficients that contain all the information related to the kinetics of the system. The final step will be to include these transport coefficients in a phase-field scheme to study the evolution of the microstructure on larger time and length scales. This multi-scale modeling process then enables to predict temperature/radiation flux conditions in which the desired microstructure is stable, and can guide the design of dedicated experiments.

(H3 oral) **Modeling of radiation-induced precipitation in an under-saturated solute solution**

D Nguyen-Manh[1], J S Wrobel[2], M Klimenkov[3] and S L Dudarev[1]

[1]Culham Centre for Fusion Energy, UK, [2]Warsaw University of Technology, Poland, [3]Karlsruhe Institute of Technology, Germany

Segregation occurring in an under-saturated solid solution driven by irradiation is a phenomenon that has significant practical implications. In this talk, a multi-scale modelling approach based on ab-initio calculations is developed where solute atoms and super-saturated vacancies (Vac) are treated as components of a multi-component alloy. The method is applied to the treatment of phase stability of W-Re-Vac using a combination of Density Functional Theory calculations, performed for more than 200 alloy structures with vacancies, and the cluster expansion (CE) method. The accuracy of the CE model is assessed against the DFT data, where the cross-validation error is less than 4.2 meV/atom. The free energy of the W-Re-Vac alloy is evaluated as a function of temperature using effective CE interaction parameters and quasi-canonical Monte Carlo simulations. In the low solute concentration range (< 5 at%Re), solute segregation occurs in the form of Re atoms decorating vacancy clusters, which are stable in the temperature range from 800K to 1600K. At lower temperatures, simulations predict precipitates with Re concentration from 30 to 50 at.%. MC simulations of Re precipitates are in excellent agreement with experimental observations performed using Atom-Probe-Tomography on self-ion irradiated W-2at.% Re alloys as well as with Transmission Electron Microscopy investigations of neutron-irradiated W samples containing up to 1.4 at.% Re accumulated as a result of neutron-induced transmutation reactions.

(H4 invited) **Multiscale modeling of the influence of semi-coherent interfaces on point defect concentrations and point defect clustering**

T Jourdan[1], A Vattré[1], H Ding[2], C Marinica[1] and M Demkowicz[2]

[1]CEA Saclay, France, [2]MIT, USA

Under irradiation, point defect supersaturation is responsible for the clustering of point defects into voids or dislocation loops. These clusters can modify the mechanical properties and lead to dimensional changes. One way of imparting radiation resistance to solids is to incorporate into them a high density of interfaces capable of absorbing and annihilating radiation-induced defects. In this work we show that elastic interactions between point defects and semicoherent interfaces lead to a marked enhancement in interface sink strength. Our conclusions stem from simulations that integrate object kinetic Monte Carlo (OKMC) with anisotropic elasticity calculations of interface stress fields. Elastic interactions of interfaces with vacancies and interstitials are characterized using elastic dipole tensors computed from first principles. Surprisingly, the enhancement in sink strength is not due primarily to increased thermodynamic driving forces, but rather to reduced defect migration barriers, which induce a preferential drift of defects towards interfaces. The sink strength enhancement is highly sensitive to the detailed character of interfacial stresses, suggesting that very efficient interfaces may be designed by optimizing interface stress fields. In addition to the evaluation of sink strengths, OKMC simulations are well adapted to simulate directly the formation of clusters. The influence of interfaces on defect clustering will be discussed.

(H4 oral) **Modeling of one-dimensional migration of interstitial clusters and their growth behavior in alpha-iron under electron irradiation**

Y Abe[1] and Y Satoh[2]

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We performed in-situ observation of one-dimensional (1D) migration of self-interstitial atom clusters and their growth behavior in alpha-iron under electron irradiation using a high-voltage electron microscopy. We found that the frequency of 1D migration was almost proportional to the damage rate by electron irradiation, and the 1D migration distance was longer for smaller clusters in specimens of higher purity, irrespective to the irradiation intensity. These findings suggest that TEM-detectable interstitial clusters are in a stationary state due to trapping by impurities and electron irradiation provides a trigger for causing 1D migration by detrapping of clusters from impurities. On the basis of the revealed 1D migration characteristics, we then extended conventional rate equations for point defect reactions under electron irradiation by taking account of trapping, detrapping, and 1D migration of interstitial clusters. The calculation of the accumulation and growth behavior of interstitial clusters showed that the saturated cluster number density decreases with lowering the impurity concentration due to a suppression of cluster nucleation rate determined by the trapping probability. It was also found that at higher irradiation doses the cluster number density turns to decrease due to the cluster detrapping induced by electron irradiation. These results well represent the evolution of interstitial clusters observed by the experiment.

(H4 oral) **Point defects in materials: measurement of elastic dipoles and polarisability effects**

C Varvenne[1], F Bruneval[2], M-C Marinica[2] and E Clouet[2]

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Point defects (PDs) in crystalline solids, such as vacancies, self-interstitials or small clusters, play a crucial role in controlling materials properties and their kinetic evolution, particularly through their interactions with other defects, like other PDs, dislocations, or surfaces/interfaces. The dipole moment representation of those defects has become a valuable tool to model those long-range interactions within continuum elastic theory, with successful applications in finite-size correction schemes, stress-driven diffusion, or sink strength optimization of semi-coherent interfaces [1-3]. Accurate measurements of elastic dipoles are needed, with a method working at the small simulation size of ab initio simulations.

Here, we perform a careful study of different methods to extract elastic dipoles from atomistic simulations: strain derivatives of the energy, adjustment on elastic displacement fields, computation of Kanzaki forces. Higher order moments in the multipole expansion and inhomogeneity effects (polarizability), that contribute to the short-range PD/defect interaction, are also considered. Empirical potentials – that allow very large simulation sizes – are used for the purpose of comparing the different methods, considering self-interstitials in hcp zirconium and substitutional constituent impurities in fcc Fe-Ni-Cr solid-solutions (defects in non-dilute random alloys). We then discuss the feasibility of the different methods within ab initio simulations, particularly with respect to their inherent technical limitations. To this end, we rely on ab initio calculations performed on the previous systems, plus self-interstitial clusters in bcc iron and vacancy in diamond silicon.

[1] C.Varvenne et al., PRB 88 (2013)
[2] T.Garnier et al., PRB 90 (2014)
[3] A.Vattré et al., NComms. (2016)

(H4 oral) **Absorption rates for cluster-dynamics modelling of mixed 1D-3D mobile species**

G Adjanor[1] and T Jourdan[2]

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For the concern of reactor life extension management, the evolution of the reactor structures materials needs to be predicted. In complement to accelerated irradiation experiments, simulation methods can provide understanding and validation on the elementary mechanisms of defects and solute interactions ruling the microstructure evolution. In cluster-dynamics methods (CD), one needs to implement in rate-equations the absorption rates (related to sink strengths) for all couples of reacting species according to their geometry and mobility, deduced from the analytical solution of the associated diffusion problem. On the other hand, in Kinetic Monte-Carlo (KMC) methods reactions between defect clusters and possibly solute elements can be quite readily implemented, once the associated energies are parameterized. It is known that in some materials, small interstitial clusters experience 1D migration, with possible rotation of their glide direction (resulting in a mixed 1D3D mobility, noted 1DR hereafter). State-of-the-art sink strength calculations account for this complex mobility but only for absorptions on a fixed sink. An adequate rate-theory modelling of defect clusters evolution should also include sink strengths for 1DR-1DR reactions, i.e. reactions between to clusters of any type mixed mobility. With the help of object-KMC, we have calculated effective values for these absorption rates depending on radii, concentrations, diffusion coefficients and rotation energies of both reaction partners. In the few analytically tractable limiting cases, the obtained dataset fits well found formulas. Finally a comparison of the outcome of the resulting CD parameterization with its OKMC counterpart will be discussed.

(H5 invited) **Mesoscale Modeling of Laser-Induced Crystallization of Amorphous Ge**

J Marian[1], L Sandoval[2] and C Reina[3]

[1]University of California Los Angeles, USA, [2]Los Alamos National Laboratory, USA, [3]University of Pennsylvania, USA

Germanium is an extremely important material used for numerous functional applications in many fields of nanotechnology. In this work, we present a mesoscale computational model of Ge recrystallization from amorphous structures after laser-spot heating. The model is centered around a phase field microstructural simulator parameterized entirely using atomistic calculations. In addition, we employ molecular dynamics (MD) simulations to supply the phase field model with mechanistic information gathered at the atomic scale. From the MD simulations, we find that crystallization occurs by the recurrent transfer of atoms via a diffusive process from the amorphous phase into suitably- oriented crystalline layers. We accompany our simulations with a comprehensive thermodynamic and kinetic analysis of the growth process, which explains the energy balance and the interfacial growth velocities governing grain growth. For the 〈111〉 crystallographic orientation, we find a degenerate atomic rearrangement process, with two zero-energy modes corresponding to a perfect crystalline structure and the formation of a Σ3 twin boundary. Continued growth in this direction results in the development a twin network, in contrast with all other growth orientations, where the crystal grows defect-free. This particular mechanism of crystallization from amorphous phases is also observed during solid-phase epitaxial growth of 〈111〉 semiconductor crystals, where growth is restrained to one dimension. We calculate the equivalent X-ray diffraction pattern of the obtained nanotwin networks, providing grounds for experimental validation.

(H5 oral) **Alloying effects on the formation of C15 interstitial clusters in iron**

L Messina[1], M-C Marinica[2], M Nastar[2], P Olsson[3] and F Soisson[2]

[1]CEA Saclay, France, [2]CEA, DEN, Service de Recherche de Métallurgie Physique, France, [3]KTH Royal Institute of Technology, Sweden

Diffusion of impurities in iron alloys plays a key role in driving the microstructure evolution during phase transformations and under irradiation. In irradiated alloys, local chemical rearrangements occur because of the thermodynamic interaction and the kinetic coupling between impurities and radiation-induced crystal point defects (vacancies and interstitials), leading to solute precipitation and segregation on grain boundaries and dislocations, thus strongly affecting the mechanical properties. Analyzing the flux-coupling tendencies qualitatively and quantitatively is therefore necessary to understand and predict the microstructure radiation response. A first objective of this work is to examine such tendencies based on first-principle calculations, determining the mobility and the diffusion mechanisms of a wide range of impurities in iron due to interaction with vacancies and interstitials.

Strain fields introduced by large defects, such as point-defect clusters and dislocations, can have a strong impact on solute-defect flux coupling. It is of particular interest to investigate the effect of the strain field induced by C15 interstitial clusters in iron [1]. Such structures are formed during displacement cascades and are predicted to be energetically favourable for small and intermediate cluster sizes. Although sessile, such clusters can grow by absorbing mobile single interstitials, which may be coupled to specific chemical impurities. The second objective of this work is to analyze how the presence of C15 complexes affects the SIA-solute flux coupling, as well as to investigate how such coupling can alter the nucleation mechanisms of these structures.

[1] M.-C. Marinica, F. Willaime, and J.-P. Crocombette, Phys. Rev. Lett. 108, 025501 (2012)

(H5 oral) **Multiscale study of plasma induced trapping of hydrogen isotopes in tungsten**

P Grigorev[1], D Terentyev[1], G Bonny[1], G Van Oost[2] and J-M Noterdaeme[2]

[1]SCK-CEN, Belgium, [2]Gent University, Belgium

Tungsten is a primary candidate material for plasma facing components in future fusion reactors. One of the current issues in the design of plasma facing component is trapping and retention of tritium since it is toxic and radioactive. Last years a extensive number of experimental studies were aimed on systematic study of mechanisms of hydrogen isotope (HI) retention in tungsten under fusion relevant plasma exposure conditions. However, the experimental data, available in literature is very scattered and does not allow one to create a physical model. Simulations of HI retention and desorption from tungsten samples with classical diffusion trapping simulation codes does not give a convincing result due to a large number of ad-hoc parameters needed to reproduce the experiment. In this work we would like to present our understanding of mechanisms governing plasma induced HI retention and material modification. Based on atomistic simulation results we propose a model of non-equilibrium HI trapping and bubble formation operating at sub-surface region of the material during plasma exposure. We link this model to classical diffusion-trapping retention mechanisms relevant for retention in the bulk of the material. The proposed model allows one to relate HI trapping with the microstructure of the material together with plasma exposure conditions. We use the model for interpretation of recent experimental results.

(H5 oral) **Shock induced phase transition in polycrystalline iron**

N Gunkelmann[1], E M Bringa[2] and H M Urbassek[3]

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Shock waves are ubiquitous in various fields of activity including physical science and engineering. They are of key interest for materials engineering, where shock-induced phase transitions may be used to harden materials resulting in a significant increase in the strength of metals.. In particular iron shows a pressure induced phase transformation from the bcc to the hexagonal close-packed phase at around 13 GPa. Here we study shock waves in polycrystalline Fe using an interatomic potential which faithfully incorporates this phase transition at the desired equilibrium pressure. Our simulations show that the phase transformation is preceded by plastic activity, giving the so-called 3-wave structure: An elastic compression wave is followed by a plastic wave which then leads to a phase-transformation front. We show that the phase transformation from bcc to hcp and vice-versa helps to drive twinning and decreases the probability of multiple spallation and crack formation. In agreement with experiments, the fracture surface is influenced by the phase transition showing smooth spall surfaces.

(H5 oral) **Modeling of out-of-local equilibrium flux couplings in dilute aluminum alloys**

T Schuler[1], T Jourdan[2] and M Nastar[2]

[1]University of Illinois, USA, [2]CEA, France

The modeling of atomic transport induced by a super-saturation of point defects in driven systems mainly uses the Onsager expression of flux couplings between point defects and atoms relying on a local equilibrium assumption. In dilute alloys, it is possible to define flux couplings in terms of mobilities and association-dissociation rates of point defect-solute clusters. Such a new cluster dynamic approach goes beyond a local equilibrium assumption. It is applied to the modeling of solute-vacancy flux coupling and subsequent solute segregation at cavities in dilute aluminum alloys quenched from high temperature. Mobilities and association-dissociation rates are deduced from ab initio vacancy jump frequencies by means of the self-consistent mean field theory and atomic kinetic Monte Carlo (AKMC) simulations. The results are then compared to direct AKMC simulations and experimental observations of solute segregation in aluminum alloys.

(H6 invited) **Formation and dissolution of protective oxide layers in a wet electrochemical environment**

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Corrosion is an inherently multidimensional problem, which involves different length and time scales, but also materials classes with dissimilar characteristics. Identifying suitable observables and modelling approaches, which facilitate understanding of corrosion mechanisms, will aid the development of strategies for protection against corrosion. Point defects in condensed phases are a feature common to each of the phases encountered within a corroding system and a very suitable descriptor from a modelling point of view. They can be treated at the level of quantum-mechanical calculations, but also allow for a seamless connection between the different phases of a corroding system via chemical potentials. This enabled us to develop an approach that unifies and “translates” theoretical concepts from the fields of semiconductor defect chemistry and electrochemistry [1], being based on a fully grand-canonical description of both ions and electrons.

Using the example of ZnO passivation layers we employ the new approach to construct defect stability phase diagrams [2], which depict the dominant native point defects of band-gap materials. We discuss which point defects control the growth and dissolution of the oxide barrier layer formed in corrosive environment and how the gained insight impacts our understanding of fundamental corrosion mechanisms [3], suggesting routes to counteract corrosion.

[1] M. Todorova and J. Neugebauer, Phys. Rev. Appl. 1 (2014) 014001
[2] M. Todorova and J. Neugebauer, Surf. Sci. 631 (2015) 190-195
[3] M. Todorova and J. Neugebauer, Farad. Discus. 180 (2015) 97-112

(H6 oral) **Hydrogen influence on diffusion in nickel from first-principles calculations**

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The diffusion coefficient of vacancy-hydrogen clusters (VHn) is calculated ab intio in Ni. The key is a good separation of timescales between H diffusion and the metal-vacancy exchange. It is shown that cluster diffusion can be treated as an uncorrelated random walk and that H is always in equilibrium before the vacancy-metal exchange. Then, the diffusion coefficient is a sum over jump paths of the equilibrium probability of being in a specific VHn configuration times the corresponding activation terms. The influence of H on the energy barrier is well reproduced by effective pair interactions between the jumping Ni and the H atoms inside the vacancy. This model is motivated by an analysis of the electronic charge redistribution in key saddle configurations. The interaction is repulsive and decreases with distance. The model is used to find easy jump path, reduce the number of saddle searches and provide an estimate of the error expected from this reduction. The application to the Ni-H system shows that vacancies are drastically slowed down by H. The effects of temperature and bulk H concentration are explored and the origin of the non-Arrhenius behavior is explained. At equilibrium, VHn clusters always induce a speed up of metal diffusion. The implications concerning H induced damage, in particular in regards to Ni-Cr oxidation, are discussed.

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(H6 oral) **Field modified diffusion in a hexagonal cell structure**

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Columnar grains prevail in many situations of planar film growth, results of a model that idealizes this structure as a lattice of identical columnar grains having a hexagonal cross-section are reported. Within this geometry, grain boundary transport of charged point defects, electrons, and holes through the film is described, while reactions with the environment constitute the boundary conditions. The model involves a self-consistent treatment of the electric fields in the three dimensional structure together with the transport equations. A C++ code, interfaced to the Trilinos project [1], has been generated to solve the coupled system of equations numerically. The model is applied to -alumina membrane oxygen permeation experiments, in which different oxygen gas pressures are applied at the membrane surfaces. Two power laws, for the permeation rates in the high and low applied oxygen gas pressure limits, have been found experimentally [2], and are compared to time dependent calculations with the developed model. The 3D model we develop here is readily adaptable to the problem of oxide scale growth.

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(H6 oral) **Multiscale thermo-chemo-magneto-mechanical modeling of polycrystalline magnetic shape memory alloys**

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Magnetic shape memory alloys (MSMA) are among the most promising alloys for designing miniature sensors or actuators. Besides stress and temperature dependence, a macroscopic deformation can be achieved by applying a magnetic field (due to some phase transition and/or some variants selection). The associated piezomagnetic effect in these materials can also be very high. On the other hand, the phase transition leads to strong heat exchanges. Due to the induced thermo-magnetic coupling, these materials are very interesting candidates to be part of a new generation of thermo-magnetic power generation devices [1].

These behaviors are strongly associated with transformations at the single crystal scale and with the magnetic domains re-organization. The development of micro-macro approaches is consequently relevant for the modeling especially when a polycrystalline medium is considered. In this paper, a multiphysics (fully coupled thermo-chemo-magneto-mechanical problem) and multiscale (magnetic domain, variant, grain and polycrystal) modeling of these materials in a multiaxial framework is presented. It uses a homogenization method and a free-energy dependent stochastic approach as a basis of a reversible constitutive law [2,3]. Hysteretic phenomena associated with nucleation/growth phenomena and with magnetization are next considered thanks to the calculation of an irreversible loading term. The macroscopic quantities at the polycrystalline scale are computed through averaging operations. Numerical results are compared to experimental results from literature illustrating the wide variety of phenomena induced by these couplings.

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(H7 invited) **Correlating disordering energetics and amorphization resistance in complex oxides**

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Complex oxides have a number of applications in nuclear energy systems and thus understanding their response to irradiation is critical for predicting performance and developing new materials. In particular, significant work has been devoted to the amorphization response of pyrochlores, a complex oxide related to fluorite that has been identified as a potential nuclear waste form. Previous work has shown a correlation between the amorphization resistance of pyrochlores under irradiation and the ease at which the cation sublattice can disorder in chemically different pyrochlores. Here, using transmission electron microscopy and x-ray diffraction, we show that the opposite behavior is observed in another complex oxide, spinels, in which amorphization resistance is inversely correlated to the ability of the cation sublattice to disorder. Using density functional theory and accelerated molecular dynamics, we attribute the different response in these two materials to structural cation vacancies that exist in spinel that facilitate kinetic pathways to relaxation that are not possible in pyrochlore. We relate the fundamentally different response in these two classes of complex oxides to how their atomic structures relate to those of their basic crystal structures, fluorite and rocksalt for pyrochlore and spinel, respectively.

(H7 oral) **Microstructural evolution of graphite under irradiation: large scale molecular dynamics simulations**

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Graphite response to irradiations has been widely studied in the past because of its importance for nuclear engineering. Although its behavior under irradiation has been widely investigated, the very details of the underlying mechanisms are still under debate and several scenarios are available [1,2,3]. With molecular dynamics simulations using empirical potentials we investigate in this paper the microstructural evolution under irradiation of two types of graphite at different length scales: (1) graphite single crystal and (2) polycristalline graphite mimicking the real nuclear graphite structure.

Primary damage was investigated by displacement cascades. While mainly point defects only survive in graphite single crystal, the nanoporosity of polycristalline graphite modifies the nature of the irradiation damage.

Dose effect was subsequently explored by means of Frenkel pair accumulations in graphite single crystal. Before amorphisation, we show that graphite single crystal follows a three stages evolution characterized by: (1) an increase of point defects (2) a wrinkling and pinning of the graphene planes at small amorphous pockets and (3) an amorphisation by percolation of the small amorphous pockets. Although each of these three stages have already been proposed [2,3], their chronology is evidenced in the present simulations [4].

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(H7 oral) **Large scale simulations of monazite-type ceramic nuclear waste forms**

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Nuclear waste management is an important issue faced by current and next generations. One of the most widely discussed solutions to it is immobilization of radionuclides in durable waste forms such as ceramics, and final disposal in a deep geological repository. In order to understand the long term performance of the ceramic waste forms we perform atomistic modeling-based characterization of these materials using ab initio and force-field simulation methods. The investigated processes include the structural and thermodynamic parameters, the phase stabilities and transitions, the defect formation energetics and the radiation damage resistance. Here we discuss the simulations of various properties of monazite-type ceramics ($LnPO_4$), emphasizing our results on the radiation damage and thermal conductivity. We simulated the primary knock-on atom (PKA) threshold displacement energies (E_d) and dislocation probabilities for the atoms in monazite. We have found that the probabilities of displacement and defect formation depend weakly on the Ln cation but strongly on the temperature. The overall result is very similar to the recent studies performed for TiO_2 (110) rutile (M. Robinson et al. Phys. Rev. B 85, 104105, 2012) . By applying the gradual defects accumulation molecular dynamics we derived the values of critical amorphization doses that closely resemble the experimental data. The subsequent quantum mechanical calculations performed on the irradiated structures allowed for estimation of the amorphization enthalpies and the entropies of the amorphous phase. We will also discuss the elastic moduli and the thermal conductivities of monazite and xenotime phosphates.

(H7 oral) **Multi-scale simulation of the experimental response of ion-irradiated zirconium carbide: role of the diffusion driven clustering of interstitials**

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The response of zirconium carbide to heavy-ion irradiation is comparable to what is observed in other non amorphizable ceramics. Indeed, below a certain threshold elastic strain builds-up with increasing fluences, then the strain is released and important dechanneling appears as well as visible TEM damage. With increasing fluence, this damage is found to spread in the material deeper than the depth of direct damaging by the ion beam. These experimental observations are reproduced and explained by Density Functional Theory informed Rate Equation Cluster Dynamics simulations (RECD). RECD aims at simulating the evolution of a population of objects through chemical rate equations, in a mean field approach.

Simulations show that the response of ZrC upon ion-irradiation is driven by the diffusion and clustering of interstitials. The apparent two-step evolution seen in experiments stems from the growth of interstitial clusters with a concomitant starvation of the smallest clusters induced by the continuous accumulation of vacancies. The damaging of the material beyond the range of primary damage is driven by the in depth diffusion of interstitials.

Beyond the case of ZrC [1], the present simulations provide a conceptual framework to understand the behavior under ion irradiation of other non amorphizable ceramics such as MgO and UO_2.

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(P2.23) **Scaling laws of cascade and sub-cascade formation in high energy ion and neutron impacts**

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In the treatment of microstructural evolution of irradiated materials, a critical aspect of the analysis is associated with the definition of the source term describing the generation of radiation defects in collision cascades. Cascade events produce clusters of defects and not just individual defects. The statistics of defect production is a necessary part of any realistic microstructural evolution model.

Computer simulations show that the defect size versus the frequency of occurrence distribution is well represented by a power law [1]. This finding is confirmed by electron microscope images of defect microstructure [2]. The outstanding question concerns the part played by cascade splitting into sub-cascades. Developing a model describing the sub-cascade splitting effect is essential for treating cascade events exceeding a certain threshold energy value.

Using a Binary Collision Approximation based model for collision cascades, we investigated the spatial repartition of the deposited energy. Using a local melting criterion, the cascades can be described in terms of separate molten subdomains. The number of subdomains as a function of the cascade energy exhibits a transition from a single domain to several subdomains. Above the cascade splitting energy the number of subdomains follows a power law, different from the power law describing the defect size distributions. The new model, combining the statistics of defect production in individual cascades with the statistics of sub-cascades, defines the defect size distributions generated by ion and neutron impacts over a broad range of cascade event energy.

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(P2.24) **Bridging the gap between atomistic and mesoscale: Statistics of the primary damage from ion and neutron irradiation**

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Computational models designed to predict the effects of neutron irradiation in future fusion reactors must be validated against available experimental results, most of which are supplied by ion irradiation experiments. Neutrons give rise to a primary recoil spectrum in the target material, and the damage production is well described by the individual cascades caused by these recoils. Self-ion irradiation experiments serve as a useful proxy, reproducing the same cascade geometry and energy density as an individual recoil from neutrons. However, a major difference between neutron and ion induced cascades is caused by the close proximity of the surface in the latter case.

Microstructural evolution models rely on an initial distribution of primary damage, which can only be obtained by statistical analysis of atomistic simulations. A key aspect influencing the evolution of the damage is the athermal formation of defect clusters occurring as a direct result of a cascade. Molecular dynamics simulations reveal that the primary damage size distribution follows a power law, and this is confirmed by *in-situ* TEM experiments in tungsten. We will present a new analytical model for the distribution of defect sizes within the primary damage, which extends the previously found power law with an explicit upper bound to the distribution, and shows good agreement with experiments. We discuss the effect of surfaces on the damage production, and highlight general aspects of the distribution, as well as material specific features, which we elucidate through a comparison of defect distributions in iron and tungsten.

(P2.25) **Kinetic rate-theory approach for helium bubble growth in irradiated RAFM steels**

B Kaiser[1], E Gaganidze[1], C Dethloff[1], D Brimbal[2], M Payet[3], P Trocellier[3], L Beck[3] and J Aktaa[1]

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Irradiation damage by neutrons in structural materials like reduced activation ferritic martensitic (RAFM) steels is an important issue for future fusion reactors. In particular the production of helium and the subsequent formation of bubbles induced by irradiation are supposed to critically influence the mechanical properties and the structural integrity of the RAFM steels. We describe the formation and growth of homogeneously distributed helium bubbles by means of kinetic rate-theory with the emission and diffusion governed absorption of mobile helium filled vacancies by bubbles, obtaining the concentration of bubbles as a function of their size. In addition to the bubble formation in the matrix, the model includes rates accounting for mobile vacancies captured by sinks such as grain boundaries. As usually in rate theory, the coefficients for absorption and emission require physical quantities passed from microscopic theories or experiments. The model is evaluated with dual beam He/Fe ion irradiations of 9%Cr-WVTa-RAFM steel (EUROFER97) performed at the JANNUS laboratory of CEA Saclay. The irradiations were carried out at temperatures of 330°C, 400°C and 500°C and induced a damage and helium concentration of up to 30 dpa and 450 He appm, respectively. The appearance and properties of bubbles are analysed with TEM technique. In agreement with the model we observe the tendency of an increasing bubble diameter with rising irradiation temperature. However, the model overestimates the size of the bubbles.

(P2.26) **Atomistic modelling of carbon diffusion in Fe-Cr alloys**

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Body centered cubic (bcc) ferritic steels such as Fe-Cr alloys present a good resistance to corrosion and to neutron irradiation damage, such as void swelling. Thus, they will be used in future fission (generation IV) and fusion nuclear reactors as structural components. Nevertheless, the presence of C in these alloys may affect the radiation induced segregation of Cr at grain boundaries and the precipitation of the Cr rich phase α', resulting in modifications of the microstructure, the mechanical properties and the corrosion resistance.

As a first step to model such complex phenomena, this study focuses on the migration of the octahedral interstitial C in the Fe-Cr-C system. As a first approximation, the diffusion of a single carbon atom in a rigid bcc lattice is considered. First, migration barriers of C as functions of local chemical environments are determined by means of Density Functional Theory (DFT). Second, a diffusion model of C fitted on the DFT calculations is developed. Third, diffusion properties and internal friction data are extracted from Atomic Kinetic Monte Carlo (AKMC) simulations of the ternary system Fe-Cr-C. These AKMC predictions are then compared to previous Internal Friction experimental data, which show that the activation energy for the diffusion of C increases non-linearly with Cr content.

(P2.27) **Evolution of defect populations in silicon carbide: coupling ab initio energetics, charged defects and rate theory**

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Ab initio based evolution of defect populations using stochastic methods or rate theory has been developed since at least a decade and has provided the explanation of the evolution of material properties of irradiated materials [1]. Its application concerns, however, mostly metals. Although applications to semiconductors or insulators exist [2], they overlook in most cases the variety of charge states of point defects. We present here an approach to overcome this limitation. First of all we compile a database of defect formation energies and energy barriers for migration and defect reactions in cubic silicon carbide, based on first principles calculations. Then we describe a way to take into account the role of charges in a homogeneous model system, and discuss in which conditions our assumptions are justified. Finally we present some results of rate theory simulations for silicon carbide under or after electron irradiation. In particular, we show examples where the mutual influence of doping and kinetics in the material matters, and we revisit our previous prediction of SiC nanodecomposition driven by vacancy-interstitial recombinations [3], where electrostatic effects were neglected.

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(P2.28) **Molecular dynamic study of structure and phase transitions in pure uranium and U-Mo alloys as metal nuclear fuel**

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Uranium has received a lot of attention due to its unique nuclear properties and its various applications in nuclear industry. In order to improve mechanical properties and corrosion resistance of uranium at room temperature while maintaining the high density, uranium is frequently alloyed with the other metals. Compared with the other high density uranium alloys and compounds, the low-enriched uranium alloys with 6-12wt.% of Mo have attracted a great deal of attention and are recognized as the most prominent candidates for advanced research and test reactors.

One should note that pure uranium has three different phases depending on temperature and pressure. Therefore, structure of uranium-based alloys (namely, U-Mo) can reflect features of different uranium phases, depending on conditions. The structural properties of body-centered cubic (BCC) and body-centered tetragonal (BCT) phases of pure uranium and U-Mo alloys are studied using atomistic simulations. The BCC lattice exhibits cubic symmetry only on the scale of several interatomic spacing's, and it is therefore more correct to denote the high-temperature state of pure uranium and U-Mo alloys as quasi-BCC. The local positions of uranium atoms in the quasi-BCC phase correspond to the BCT structure. This fact is the possible origin of the difficulties encountered in the description of the BCC phase of pure uranium by *ab initio* methods that have been a challenge for researchers for decades.

(P2.29) **Atomistic modelling of pre-melting and melting UO2 , UN2, TiH2 Korneva M.A.1,2 , Starikov S.V.1,2**

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Fluorite type structures can show superionic transition at temperatures close to melting. There are certain difficulties in constructing the theory of superionic transitions. Nevertheless, the mechanism of this transition in fluorites is well known — the phenomenon is provided by the growth of concentration of point defects in anion sublattice. There still remain a number of fundamental questions: whether the superionic transition actually can be considered as a phase transition, to which type this phase transition belongs, and what are the necessary conditions for the observation of this transition. The process is characterized by high growth of electric and heat conductivity, and some theoretical approaches to describe this transition can explain this effect.

In this work the results of the atomistic simulation of a superionic transition and melting of stoichiometric UN_2, UO_2 and TiH_2 have been presented. The temperature dependences of defects' concentration in the anion sublattice and leaps of the heat capacity and isothermal compressibility have been calculated in UO_2 and TiH_2. It has been shown that the curve of the superionic transition in the *PT*-diagram can be described by the Ehrenfest equation. The possibility of describing the superionic transition within the framework of the theory of second-order phase transitions has been discussed. The conditions of the existence of superionic transition have been discussed.

(P2.30) **A multiscale model of lithium-ion cell dynamics with thermal effects**

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The contribution presents computational results obtained by a one-dimensional mathematical model of the Li-Ion cell dynamics based on first principles describing the ion diffusion through the electrolyte, electric potential distribution, Butler-Volmer kinetics, and the thermal effects occurring during charge-discharge cycles of the battery. The numerical model is obtained by the FVM discretisation of the governing laws, appropriate coupling of the model parts and upscaling from the electrode grain size to the electrode macroscale. The model is devoted to optimization of the battery life cycle under extreme loading.

(P2.31) **Coupled micromagnetic/ phase field modelling of magnetic shape memory alloys – scale effect**

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Our time is highly characterized by the use of increasingly widespread electromagnetic actuators, from larger to smaller scales. The development of efficient micro-actuators through the development of new materials is relevant, using for example the pseudo-elasticity of Shape Memory Alloys (SMA). The SMAs belong to the family of materials whose behaviour is characterized by an austenite-martensite phase transformation. This transformation can be activated by heating or cooling and/or mechanical stress. Among the SMAs, Magnetic Shape Memory Alloys (MSMAs) are furthermore ferromagnetic. Under the action of a magnetic field, through the existence of a magnetostatic coupling as well as a magneto-mechanical coupling a phase transformation and/or a reorientation of martensite variants can occur. The behaviour of these alloys is dependent of the amount of stress, temperature and/or magnetic field applied. Modelling the behaviour of these complex alloys remains difficult but essential in order to determine and predict their response under complex loadings (multiaxial, heterogeneous) and extend their application range.

In this work, a coupled micromagnetic / phase field finite element modelling of MSMAs in a multiphysics framework with strong couplings (chemo-thermo-magneto-mechanical) is proposed in order to take the evolving nature of the microstructure into account. One of the main difficulties for the implementation of this model is the consideration of the exchange effects (defining both the domain walls and phase interfaces thickness), which are highly size and therefore mesh dependent.

(P2.32) **Molecular dynamics study of the formation of martensite in Fe-C systems**

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Atomistic simulation methods such as molecular dynamics (MD) can shed light on the mechanisms controlling the phase transformation from austenite to martensite in pure Fe and Fe-C systems. The thorough understanding of this phase transformation is important to further improve the properties of advanced high strength steels. We will evaluate the effect of carbon concentration and temperature on the martensitic transformations in single crystal and nanocrystalline Fe-C systems. The simulations will capture the main features and mechanisms of nucleation, growth, and pathways of martensitic transitions. This study will help answer the questions such as how does carbon affect the nucleation and growth of martensite transformations at atomic scales which can be difficult to analyse experimentally.

(P2.33) First principles study of Cu impurity diffusion in TiN

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One of the important elements in microelectronic devices is the diffusion barrier whose role is to prevent copper interconnects from contacting silicon. TiN is known to perform well as a diffusion barrier, however, there is little known about atomistic processes underlying the excellent performance of TiN. Experimental measurements of the Cu diffusion coefficient in TiN and the determination of the diffusion mechanism are normally difficult to perform and the interpretation of the results can be rather ambiguous due to the extremely slow diffusion of Cu in TiN. Moreover, a rather high degree of TiN off-stoichiometry as well as the presence of grain boundaries in the material makes interpretation of the results even more complicated. Here, theoretical modelling based on first-principles calculations can provide a detailed description of Cu diffusion and can be applied for a better understanding and an improved interpretation of the existing experimental data. In this work, we consider two mechanisms of Cu impurity diffusion in TiN, namely interstitial and vacancy-mediated diffusion on both nitrogen and titanium sublattices. Using density functional theory calculations, we consistently include the influence of the off-stoichiometry within the dilute solution model and incorporate temperature effects on the diffusion of Cu within the quasi-harmonic approximation. We obtain a diffusion coefficient which not only agrees well with most of the available experimental data, but we also suggest a possible mechanism of atomic Cu diffusion operative at elevated temperatures and provide a deeper understanding of the barrier properties of TiN against copper diffusion.

(P2.35) Development of an object kinetic Monte Carlo model for the microstructure evolution of neutron-irradiated reactor pressure vessel steels

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Radiation-induced embrittlement of reactor pressure vessel steels is one of the most important lifetime limiting factors of existing nuclear power plants. The primary mechanism of embrittlement is the obstruction of dislocation motion produced by nanometric defect structures that develop in the bulk of the material due to irradiation. In this work we developed a full object kinetic Monte Carlo model able to simulate the microstructure evolution at ~300°C for two types of steels, an Fe-C-MnNi model alloy and a high-Mn, high-Ni RPV steel representative of the Swedish pressurized water reactors at Ringhals, subjected to different neutron fluxes. The model pursues a “gray-alloy” approach, where the effect of solute atoms is introduced by modifying the parameters that govern the mobility of defect clusters with an explicit dependence on solute concentrations. The slowing down of SIA clusters can be justified in terms of interaction between solutes and crowdions in Fe, while the substantial immobilization of vacancy clusters above a certain size (~10 vacancies) was verified by means of independent atomistic kinetic Monte Carlo simulations and proved to be essential to satisfactorily match with the material experimental characterizations. Specific reference neutron irradiation conditions were successfully reproduced, while the dose-rate showed to play a relevant role on the microstructure evolution with a predominance of single defects and smaller defect clusters at lower fluxes. Finally, the SIA density predicted matched the experimental solute-cluster density observed in APT, thereby suggesting that MnNi-rich nanofeatures might form as a consequence of solute enrichment on immobilized small interstitial loops.

(P2.36) An atomistic approach to Al-Mo-U alloys through MEAM classical potentials

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U-Mo alloys dispersed in an Al matrix are a prototype of nuclear fuel for new experimental reactors. Interdiffusion and reaction between components promote the formation of intermetallic phases. Under irradiation conditions, the generated interaction layer suffers an increasing porosity that gradually degrades the material properties. Intermetallic formation and their kinetics in these alloys have been identified and studied in specifically designed diffusion experiments [1]. However, it is also necessary to have theoretical models to help determine the processes that occur at the atomic level.
In this work, appropriate interatomic potentials of the MEAM type [2] for the Al-Mo-U system are presented. Potentials for pure elements are able to reproduce cohesive and structural characteristics of these metals as well as various point defect properties. Such potentials are then used to find appropriate interactions for the three binary alloys of the ternary system. These cross element potentials reproduce reasonably well the lattice parameters and formation energies for the experimentally observed intermetallic phases in each binary system. Their stability against most common metastable phases is also taken into account. The thermal behaviour of such potentials is evaluated by molecular dynamics simulations. Growth of the Al_3U intermetallic is obtained in an Al/U interface, in agreement with the experimental evidence.

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(P2.37) Optimization of an AKMC model to simulate the long-term nanostructural evolution of pressure vessel steel under irradiation

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Radiation-induced embrittlement of reactor pressure vessel is a limiting factor for a potential life extension of the nuclear power plant. Since this component is not replaceable, understanding the long-term evolution of its microstructure is a major challenge. Experimental observations have shown that the formation of rich-solute cluster under irradiation contributes to the changes in mechanical properties evolution. However, the elementary mechanisms leading to their formation are still an open question.

Predicting the formation of these nano-features requires to start from an atomic description of the system. Atomic Kinetic Monte Carlo (AKMC) is a method fit to treat systems governed by diffusion. It takes into account elementary events occurring at the atomic scale and is thus able to describe precisely the microstructure evolution. Unfortunately, this method requires very long calculations and simulations in service condition are not yet possible. Strategies used to speed up the simulations by two orders of magnitude will be exposed. Furthermore, improvements of the AKMC parameterization based on recent ab initio calculations will be presented. High dose simulated microstructures will also be compared to experimental results.

(P2.38) **First principles simulation of Be and Be12Ti as candidate materials for neutron multiplier**

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Beryllium is considered as a candidate material for neutron multiplier in the fusion blanket of ITER. At the same time intermetallic beryllium compounds possessing higher melting point, lower chemical reactivity and lower swelling are considered as alternative neutron multiplier materials for DEMO. In this work we try to understand the origin of the superior properties of titanium beryllide by performing comparison of various properties of pure Be and $Be_{12}Ti$ alloy using density functional theory (DFT).

Lattice parameters and elastic moduli of $Be_{12}Ti$ at 0 K were calculated for the tetragonal structure, which was recently shown to be the only stable structure of this compound. This structure was not investigated via DFT methods before.

$Be_{12}Ti$ is produced by mutual diffusion of the components. Therefore we estimated various migration barriers for Ti in Be and Be in Ti using nudged elastic band method.

For tritium retention and release, tritium binding energies with vacancy are essential. In the present work isotope effects on binding were neglected, hence hydrogen instead of tritium was simulated. The dependences of binding energy on the number of hydrogen atoms in vacancy of Be and $Be_{12}Ti$ were calculated. It was revealed that hydrogen binding energy is lower in $Be_{12}Ti$ and tritium release should occur faster and easier than that in Be.

This study shed light on the origin of the advanced properties of $Be_{12}Ti$ on atomic scale.

(P2.39) **First principles and molecular dynamics determination of the threshold displacement energy in beryllium**

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Beryllium is a neutron multiplier material for tritium breeding blanket in the future fusion reactor, where it will be subjected to neutron irradiation. The neutron induced damage is commonly estimated using the so-called NRT standard, which supposes that the damage is inversely proportional to the threshold displacement energy, E_d. For several materials this value was determined experimentally, but an 'educated guess' is used for the others. Unfortunately, often the experimental values are quite different from these guesses. E.g. the existing experimental data for Be suggest significantly lower E_d value (< 10 eV) than that commonly used (31 eV).

The value of E_d is often estimated from MD simulations of collision cascades. However, such predictions are sensitive to the empirical interatomic potentials employed. The idea of this work is to compare, how much different can be the 'true' threshold damage energies calculated using first-principles approach and an empirical potential. For that, we use a straightforward method of the displacement energy determination that has already been applied for other materials (e.g. Si, W, etc.). Namely, E_d is determined as an orientational average of displacement thresholds for recoils ejected in different lattice directions in dependence of lattice temperature. Assuming that an apparent displacement threshold in cascade simulations is proportional to the 'true' one, this approach can be used for scaling the potential-based MD damage predictions, opening a way for more reliable calculations of displacement damage in metals.

(P2.40) **Multiscale approach to the determination of damage from fast neutrons in beryllium**

V Borodin[1] and P Vladimirov[2]

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The determination of the primary damage in metals due to fast neutron irradiation is a complicated problem. First of all, the majority of atoms are displaced not by neutrons themselves, but by primary recoils (PKAs). Second, PKAs have energies of hundreds of keV and create cascades of atomic collisions, producing both single Frenkel pairs and dense subcascades. Traditionally, the in-cascade displacements are calculated using binary collision approximation, which is unreliable for dense subcascades. Alternatively, the binary collision approximation can be used for counting single Frenkel pairs only, whereas the secondary recoils able to produce localized cascades are counted, but not followed explicitly. The displacement production in dense cascades is then determined independently using molecular dynamics simulations. Combining contributions from different calculations, one gets the total number of displacements created by particular neutron spectrum.

Here this program is applied to Be irradiation in a fusion reactor. For this particular neutron spectrum we estimate the energy spectrum of primary recoils, calculate the total numbers of single Frenkel pairs per incident neutron and the energy spectrum of secondary recoils in the 'dense cascade' energy window (0.5 to 3 eV). The latter spectrum can be further converted into the number of created point defects using the results of our earlier MD simulations of cascades in Be. We demonstrate, that the contributions to the total damage from single Frenkel pairs and dense cascades are comparable. It is expected that the suggested approach opens a way for more reliable calculations of displacement damage in neutron-irradiated metals.

Symposium I

(I1 invited) **Multi scale modeling of block polymers for applications in patterning**

J de Pablo

University of Chicago, USA

Block copolymers are being considered as viable candidates for commercial-scale applications in nanoscale patterning. In this context, the overall aim is to control the morphology of ordered block polymer phases at length scales of nanometers, and to achieve absolute perfection in the resulting structures. Important questions arise in these applications. On the one hand, models must be developed capable of describing equilibrium morphologies as well as relevant metastable states. On the other hand, the dynamics of these materials must also be described accurately in order to arrive at reliable descriptions of the assembly process. In this talk, I will describe a multiscale formalism that has been particularly useful for design of block polymer directed assembly strategies, including prediction of the morphologies that arise in thin films and the kinetics of morphology formation, as well as for interpretation of scattering data over large areas. More specifically, I will describe the models and their application to diblck and multiblock materials, both in the bulk and thin films, I will discuss a slip-link formalism for treatment of entangled dynamics, whose results will be compared to those of fine-grain models, and I will describe efforts to interpret massive CDSAXS and GISAXS data sets in terms of evolutionary strategies that rely on our physics-based models.

(I1 oral) **Molecular mechanisms of plastic deformation in sphere-forming thermoplastic elastomers**

J Rottler and A Parker

University of British Columbia, Canada

Nanostructured block copolymers are structurally heterogeneous materials, whose mechanical properties are controlled by molecular level mechanisms at interfaces. We employ multiscale molecular dynamics simulations to investigate deformation and plastic flow of such polymers. We focus on models for the canonical case of sphere-forming triblock elastomers, where chain ends embedded in glassy spheres effectively cross-link a rubbery matrix. The spherical morphology of the copolymers is obtained in simulations of polymers with soft potentials to speed up the phase separation dynamics [1], while plastic deformation is studied after fine-graining to a bead-spring model with matching chain conformations and thermodynamics. The evolution of the spherical morphology and chain conformations are compared for different deformation protocols and polymer molecular weight, and the consequences for the macroscopic stress-strain response will be discussed [2]. Our simulations reveal cavitation at different stages of deformation, analyze the role of entanglements during deformation and permit quantitative tests of the predictions of common network models for block copolymer elasticity.

[1] A. J. Parker and J. Rottler, Macromolecular Theory and Simulations 23, 401 (2014)
[2] A. J. Parker and J. Rottler, Macromolecules 48, 8253 (2015)

(I1 oral) **Modelling polymer deformation during 3D printing**

C McIlroy and P Olmsted

Georgetown University, USA

3D printing has the potential to transform manufacturing processes as we know them, yet improving the strength of printed parts, to equal that of traditionally-manufactured parts, remains an underlying issue. The most common method, fused deposition modelling, involves melting a thermoplastic, followed by layer-by-layer extrusion of the molten viscoelastic material to fabricate a three-dimensional object. The key to the ensuring strength at the weld between these layers is successful inter-diffusion.

However, as the printed layer cools towards the glass transition temperature, the time available for diffusion is limited. In addition, the extrusion process can significantly deform the polymer micro-structure prior to welding and consequently affect how the polymers “re-entangle” across the weld. In particular, polymer alignment in the flow can cause de-bonding of the layers, creating defects in the final printed object.

We have developed a simple model of the non-isothermal printing process to explore the effects that typical printing conditions and material rheology have on the polymer micro-structure. In particular, we incorporate both the stretch and orientation of the polymer using the Rolie-Poly constitutive equation to examine how the melt flows through the nozzle and is deposited onto the build plate. Furthermore, the mechanism by which the resulting non-linear deformation relaxes influences the welding characteristics.

(I1 oral) **Bridging the gap between molecular and macroscopic models of the mechanics and dynamics of anisotropic fluids**

P Ilg

University of Reading, UK

Liquid-crystals, dipolar fluids and polymers are examples of complex fluids that show strong anisotropic properties when subjected to external perturbations like flow fields. On a molecular level, these fluids are successfully described by mechanical models of interacting many-particle systems obeying Newtonian dynamics for translational and rotational degrees of freedom, whereas different, macroscopic models are typically used on long-time and large-length scales.

While so far the relation between molecular and macroscopic models has remained largely unclear, we here use a systematic method based on projection operators and nonequilibrium statistical thermodynamics in order to connect both levels of description.

For the example of nematic liquid-crystals, we (i) identify the molecular mechanisms relevant for the macroscopic behavior of interest, (ii) determine the parameters and transport coefficients of the macroscopic model, and (iii) suggest improvements on current macroscopic models.

(I1 oral) **Coarse-grained molecular dynamics simulation of amorphous polymers under multiaxial loading**

Y Umeno and A Kubo

University of Tokyo, Japan

Polymer materials are promising for industrial applications including structural materials in automobiles and airplanes. Numerical simulations based on macroscopic models such as the finite element method (FEM) are being carried out as they are essential for efficient designing. One of the major challenges in computational simulation of polymers is the difficulty in constructing appropriate constitutive laws in continuum modeling. For better and more reliable numerical simulations, more sophisticated construction of material models is demanded. As an effort to overcome this problem, we make multiscale simulation using coarse-grained atomistic models in a bottom-up fashion. Focusing on amorphous polymer materials, we start from all-atom molecular dynamics (MD) to coarse-grained MD, trying to establish the constitutive law to describe deformation behavior and fracture criteria. We devised a modeling scheme of constructing energy functions used in the coarse graining model. In the study we put emphasis on the effect of multiaxial loading conditions on deformation and fracture behaviors, which is crucial to establish a sophisticated material model.

(I2 invited) **Simulating mechanical properties of nanostructured polymers with coarse grained models**

J-L Barrat

Université Grenoble Alpes, France

I will present results on mechanical properties of solid polymer materials obtained using simple corase grained models. These models do not describe the molecular details, and keep only the main features of the polymeric material: chain connectivity, heterogeneity in elastic properties. I will discuss how the mechanical response varies depending on the nanostructure, taking as examples amorphous polymers, lamellar block copolymers or semi crystalline homopolymers.

[1] Plastic Deformation Mechanisms of Semicrystalline and Amorphous Polymers, S. Jabarri-Farouji et al ACS Macro Letters, 2014

[2] Nanoscale Buckling in Lamellar Block Copolymers: A Molecular Dynamics Simulation Approach, A. Makke et al, Macromolecules, 2013

(I2 oral) **Effect of network structure on fracture process of double-network gels by coarse-grained molecular dynamics simulation**

K Saito, Y Ootani, T Nishimatsu, Y Higuchi, N Ozawa and M Kubo

Tohoku University, Japan

Polymer gels have good biological compatibility. For example, they are good candidates for artificial joints. However, it is difficult to apply polymer gels to artificial joints because they are too brittle to use in human bodies. Recently, remarkable toughness double-network (DN) gels were developed. Typical DN gels consist of highly cross-linked poly 2-acrylamido-2-methylpropanesulfonic acid gel (PAMPS) and slightly cross-linked poly acrylamide gel (PAAm). To develop high performance and toughness gels, it is essential to reveal effects of two kinds of polymer chains. Thus, we examine a fracture process of DN gels by coarse-grained molecular dynamics simulation.

We develop a modeling method for DN gels and then stretch the DN gel model. During stretching, PAMPS begins to dissociate at a strain of 1.0, and the stress increases. At strains from 4.0 to 5.0, PAAm simultaneously dissociates and the stress decreases. Then, the dissociation of PAMPS stops and only PAAm dissociates at a strain of 12.0, while the stress remains almost the same. We reveal that DN gels gradually exert PAMPS and PAAm characteristics.

Next, we change the chain length and tension to reveal their influence on the mechanical properties. DN gels containing longer PAAm chains exhibit higher fracture strength because many entanglement points made by longer chains deconcentrate stress. When a PAMPS network is tense, Young's modulus increases because a tense network is hardly deformable at low strain. We reveal that longer slightly cross-linked network chains and a tense highly cross-linked network are important for the mechanical strength.

(I2 oral) **Inter-particle forces beyond the classical DLVO theory**

C Labbez, G Guillaume and M Turesson

ICB UMR 6303 CNRS, France

In the realm of colloid science inter particle forces play a key role in the control of colloidal stability and in the design of self-assembling bulk materials with predefined properties. The rationalization and prediction of these forces is thus of great interest. In 1941, Dejarguin and Landau were the first to develop a quantitative theory to explain the aggregation of aqueous colloidal dispersions and to describe the force between charged surfaces interacting through a liquid medium. Seven years later, Vervey and Overbeek arrived independently at the same result that forms today the basis of the so-called DLVO theory. Although very successful, this theory presents some limitations. Probably, the best known is its neglect of ion-ion correlations which, in systems containing highly charged particles and multivalent counterions, induced strong electrostatic short range attractions. Another important but often forgotten limitation is its restriction to the ideal thermodynamic limit, i.e. very dilute systems. In my presentation I will present examples to illustrate and propose solutions [1] to overcome these limitations.

[1] Martin Turesson, Bo Jönsson, and Christophe Labbez, Langmuir, **2012**, *28*, 4926–4930
[2] Axel Thuresson, Magnus Ullner, and Martin Turesson, J. Phys. Chem. B, **2014**, *118*, 7405–7413

(I2 oral) **Continuous-discontinuous long fiber-reinforced polymer structures: Modeling, characterization and validation**

T Böhlke, FHenning, L Kärger, T Seelig and K A Weidenmann

Karlsruhe Institute of Technology (KIT), Germany

Discontinuous long fiber-reinforced polymer structures with local continuous fiber reinforcements represent an important and new class of lightweight materials. This class of materials has a significant potential for energy savings due to the high specific stiffness and strength as well as the variety of design options in diverse technical applications, e.g., in vehicle construction. In contrast to the continuous fiber-reinforced composites of non-crimp or woven fabrics, there is still a lack of integrated and experimentally proven concepts for the manufacturing, modeling and dimensioning of combinations of discontinuously and continuously reinforced polymer structures. Especially in the field of application of three-dimensional load-bearing structures, there is considerable demand for the enhancement of scientific methods. In the talk, long fiber reinforced sheet molding compounds (SMC) and thermoplastics (LFT) are considered. The compression molding process is analyzed by in-mold rheological measurement and modeled by different (macroscopic) approaches for fiber interaction and viscosity. X-ray computed tomography is used for the analysis of the composite's microstructure as well as to determine fiber orientation tensors and fiber length distributions. Additionally, the data is used for both mean field homogenization as well as full-field simulations. The full-field modeling as well as experimental data are used to evaluate the different mean field approaches. The effective directional dependent material behavior of LFT and SMC is investigated by mechanical testing including biaxial loads.

(I3 invited) **Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modeling coupled with NEMD simulations**

P Stephanou[1], D Tsalikis[2] and V Mavrantzas[2]

[1]ETH Zurich, Switzerland, [2]University of Patras, Greece

Polymer matrix nanocomposites (PNCs) are formed by adding nanoparticles (NPs) to a polymer matrix. In the present work we develop a multiscale approach to study the rheology of PNCs with spherical inclusions by interfacing rheological models with non-equilibrium molecular dynamic simulations (NEMD). The basis of our work is a mesoscopic rheological model for PNCs derived in the framework of the Generalized Bracket formalism of nonequilibrium thermodynamics. The model was initially developed for unentangled PNCs and showed a very promising comparison with experimental data regarding the phase behavior and rheological properties of these materials in shear. In the absence of chain elasticity, it reduces to the Jefferey constitutive equation for the rheology of a Newtonian suspension of NPs. Next, it was extended to entangled polymer melts guided by the model proposed by Marrucci-Ianniruberto for describing flow-induced chain orientation and stretching in strong flows. In a second step, atomistic NEMD simulations are carried out with model PNCs samples similar to those used in experimental studies in order to get estimates of the values of the parameters appearing in the mesoscopic model. Key among these parameters is the polymer chain relaxation time and its dependence on the volume fraction of NPs. Additional parameters refer to the degree of interaction between polymer chains and NPs or between NPs and NPs. Our combined theoretical-simulation work provides a unified approach to the phase behaviour, chain conformation, swelling and rheological properties of PNCs melt, as a function of NP volume fraction, NP size, and imposed deformation rate.

(I3 oral) **Simulation of viscoelastic flows via Smoothed Particle Hydrodynamics combined with the Discrete SlipLink Model**

J D Schieber[1], H Feng[1], M Andreev[2] and E Pilyugina[1]

[1]Illinois Institute of Technology, USA, [2]University of Chicago, USA

We present a numerical method for prediction of complex viscoelastic flows based on a combination of stochastic simulation via a high-fidelity slip-link model, and macroscopic simulation using smoothed-particle hydrodynamics (SPH). The macroscopic transport equations are solved using SPH consistently with the stresses calculated using the discrete slip-link model for an ensemble of chains in each particle. The polymer model (DSM) uses only a single adjustable parameter whose value is determined from equilibrium stress relaxation, whereas all other parameters are determined from atomistic simulation. Given the strong connections of the underlying molecular model to an atomistic description, nearly *ab initio* predictions of complex processing are feasible. We performed several tests to show that the proposed technique allows for accurate predictions in feasible computational time for non-trivial flow geometries with different chain architectures or flows of blends of branched and polydisperse linear chains.

(I3 oral) **Multiscale modelling of buckling in thin polymer films and characterization by molecular dynamics**

F Detrez[1], Y Cong[2], H Zahrouni[2], and J Yvonnet[1]

[1]Université Paris Est, France, [2]Université de Lorraine, France

A multiscale model of thin polymeric films is constructed and characterized by molecular dynamics simulations. For this purpose, a continuum shell-like model is employed to investigate buckling of polymeric films. The elastic coefficients of shell model are identified by MD simulations on elementary cell of linear monodisperse polyethylene. In the context of small strains, the local solution on this elementary cell can be decomposed into six strains and six-strain gradient modes, associated with corresponding boundary conditions [1]. The heterogeneities can have arbitrary morphology but are assumed to be periodically distributed in the tangential direction of the shell. In order to deal with instabilities with improved efficiency and robustness, the extension of the small-strain framework to geometrical nonlinearities are solved by a FEM discretization with a perturbation approach. The procedure is purely sequential and does not involve coupling between scales. The continuum model is compared to the full MD simulations.

[1] Y. Cong et al. (2015) Int. J. Numer. Meth. Engng; 104: 235–259

(I3 oral) **Minimalist two-scale model for the viscoelastic behavior of elastomers filled with hard nano-particles**

M Hütter[1], M Semkiv[1]and D Long[2]

[1]Eindhoven University of Technology, Netherlands, [2]CNRS, France

A dynamic two-scale model is presented for describing the mechanical behavior of elastomers filled with hard nanoparticles, particularly the Payne effect and the Mullins effect. According to literature, both of these effects have their origin in the constraint-induced vitrification of the matrix material between neighboring filler particles, leading to so-called glassy bridges. Yielding of the latter amounts to the Payne effect, while physical aging of the glassy material gives rise to the Mullins effect. Many-particle models have been developed to describe the mechanical behavior of such composites [Merabia et al., Macromolecules 41, 8252-8266 (2008); Merabia et al., J. Polym. Sci. Pol. Phys. 48, 1495-1508 (2010); Papon et al., Macromolecules 45, 2891-2904 (2012)]. For computational efficiency and in view of macroscopically inhomogeneous deformations, we strive in this contribution to reduce the model complexity drastically, while keeping the essential physics in the model. Using nonequilibrium thermodynamics, we propose a dynamic two-scale model that couples continuum mechanics with the dynamics of a single representative particle-pair on the meso-scale. This reduced model is studied numerically in oscillatory deformation. The resulting stress-strain response (Payne effect) is compared to the many-particle model in the literature, and benefits as well as short-comings of the new approach are discussed. Finally, it is discussed how the physical aging of the glassy bridges (Mullins effect) can be incorporated, using the concept of kinetic/vibrational and conformational subsystems, akin to two-temperature models in the literature.

(I4 invited) **Micromechanics of semicrystalline polymers: towards quantitative predictions**

H van Dommelen[1], M Poluektov[2], A Sedighiamiri[3] and L Govaert[1]

[1]Eindhoven University of Technology, Netherlands, [2]Uppsala University, Sweden, [3]SABIC Innovative Plastics, Netherlands

The mechanical response of a polymer material, including the mode of failure and the time-scale on which it occurs, is strongly influenced by the processing conditions. This is particularly true for semicrystalline polymers in which structural features, such as the degree of crystallinity, crystal type, size and orientation, that strongly influence their mechanical properties, may vary drastically depending on subtle details of the manner in which the polymer is shaped into the final product. During processing of a material, often an oriented microstructure is formed, leading to anisotropic properties. To improve product performance, a fundamental and quantitative understanding of how anisotropic properties, including yield and failure kinetics, depend on the structure is required.

A micromechanical model that describes the macroscopic response as a function of the morphological structure and constitutive properties of the constituents has the potential to form a predictive tool for the macroscopically anisotropic properties of a semicrystalline polymer with a processing-induced microstructure. Initially, the application of micromechanical models has been mostly limited to macroscopically isotropic structures and was aimed at obtaining a qualitative description of the mechanical response. Recent research has focused on improving the quantitative abilities of a multiscale micromechanical model, in particular for the stress-dependence of the rate of plastic deformation, i.e. the yield kinetics, also for oriented material. In this presentation, an overview is given of the development of the so-called composite inclusion model for semicrystalline polymers from first being a qualitative model, towards a model that quantitatively predicts the response of these materials.

(I4 oral) **Tensile deformation of amorphous and semicrystalline polymers**

S Jabbari-Farouji[1], J Rottler[2], O Lame[3], A Makke[4], M Perez[3] and J-L Barrat[5]

[1]University of Mainz, Germany, [2]University of British Columbia, Canada, [3]INSA Lyon, MATEIS, University of Lyon, France, [4]Institut Charles Delaunay, France, [5]Universtiy of Joseph-Fourier, France

To gain an insight into underlying mechanism of deformation in solid-like polymers, we employ large-scale molecular dynamics simulations. We compute the uniaxial tensile response of amorphous and semicrystalline states of a crystallizable bead-spring polymer model [1]. Our simulations allow us to observe directly the mechanisms of plastic deformation of semicrystalline states on the length scales stretching from the lamella thickness to scales beyond the size of crystalline domains. We address two key questions: i) How do ordered and amorphous regions transform under uniaxial tension? ii) How do mechanical properties of semicrystalline polymers differ from their amorphous counterparts above and below the glass transition temperature?

We find that at relatively small deformations, the hard crystalline skeleton dominates, whereas the entangled amorphous network is predominant in the strain-hardeningregime as amorphous polymers reorient along the tensile axis [2,3]. In oder to establish structure-property relations for uniaxial response, we perform a systematic study of dependence of flow curve, Young's modulus and strain-hardening stiffness on polymer's length. We discuss the effects of density of tie molecules and entanglements on the mechanical response.

[1] H. Meyer and F. Muller-Plathe, J. Chem. Phys. 115, 7807 (2001)
[2] S. Jabbari-Farouji, J. Rottler, M. Perez, O. Lame, A. Makke & J.-L. Barrat, ACS Macro Lett. 4, 147 (2015)
[3] S. Jabbari-Farouji, J. Rottler, M. Perez, O. Lame, A. Makke & J.-L. Barrat, J. Phys.: Condens. Matter 27, 194131 (2015)

(I4 oral) **Polymer mechanical spectroscopy using coarse-grained molecular dynamics**

M Mahaud[1], J Morthomas[1], L Chazeau[1], M Perez[1], C Fusco[1] and G Marque[2]

[1]Laboratoire INSA Mateis, France, [2]EDF, France

In this study, a coarse-grained molecular dynamics model have been used to create elastomer networks. In this model, popularized by Kremer & Grest, weak bonds between chains are generated by a Lennard-Jones potential and covalent bonds in chains, as cross-links, are represented by non-crossable bonds. A radical-like polymerization algorithm have been used to generate homopolymer melts for several chain lengths, shorter and longer than the entanglement length. A cross-linking algorithm have been developed and used to randomly and homogeneously cross-link these melts. The resulting samples have been submitted to cyclic low-deformation tests at various temperatures to study their visco-elastic behavior. The alpha-relaxation is well reproduced and disentanglements are observed for very high temperatures for polymer melts and not for their cross-linked counterparts. It is finally demonstrated that he weak bond cut-off radius radius affects the disentanglement for high temperatures.

(I5 invited) **Fluid flow and percolation in elastic contacts**

M Müser

Saarland University, Germany

Fluids no longer leak through the thin gap between a nominally flat, rigid substrate and an elastic seal when the seal is squeezed with a sufficiently large load or adhesion against the surface. The resistance to fluid fluid flow through such a gap is studied below and near the sealing transition using computer simulation. In contrast to seemingly related percolation models, the critical flow near the sealing threshold turns out relatively independent of the multi-scale channel topography. Instead, the last constriction determines the overall resistance to flow. Competing theories and numerical strategies to tackle the given problem are presented.

(I5 oral) **Multiscale phenomena in filament networks: What is common with buckypaper and cell division**

M Karttunen[1] and J Astrom[2]

[1]Eindhoven University of Technology, Netherlands, [2]Finnish IT Center for Science, Finland

Fiber networks are ubiquitous in nature. For applications, network structure offers the possibility to design strong and light materials via tuning, e.g., strength, conductivity, and optical properties. In biology, the cytoskeleton is perhaps the most spectacular example of filament networks: It allows for cell division to occur by dynamically adjusting the degree of cross-linking (by molecular motors) depending on the degree of external and internal stresses. We discuss a full three-dimensional network model that includes molecular motors. We demonstrate that filament networks show formation of stress fibers, strain hardening, aster formation [1] and that they display a texture dependent secondary stiffness transition [2]. The latter appears to offer the possibility to tune network response in a new way via texture design. We also demonstrate that from a mechanistic point of view, cell division does not require polymerization [3]. Such systems are inherently multiscale and we demonstrate that our model captures the relevant phenomena.

[1] Åström, J. A.; Kumar, P. B. S. &, Karttunen M. Aster formation and rupture transition in semi-flexible fiber networks with mobile cross-linkers. *Soft Matter,* 2009, 5, 2869-2874

[2] Åström, J. A.; Sunil Kumar, P. B. & Karttunen, M. Stiffness transition in anisotropic fiber nets. *Physical Review E,* 2012, 86

[3] Åström, J. A.; von Alfthan, S.; Sunil Kumar, P. B. & Karttunen, M. Myosin motor mediated contraction is enough to produce cytokinesis in the absence of polymerisation. *Soft Matter,* 2010, 6, 5375

(I5 oral) **Chemo-mechanical coupling in shape memory polymers: Theory versus experiment**

F Varnik, E Mahmoudinezhad, A Marquardt, K Neuking and G Eggeler

Ruhr-Universität Bochum, Germany

Shape memory polymers are fascinating materials, which are able to recover large shape changes. They often find applications in harsh chemical environments which deteriorate their mechanical properties and reduce their life time. The degradation of shape memory polymers can be qualitatively and quantitatively characterised considering their long-term functional behaviour in liquids and gaseous environments. Chemical degradation of polymer materials is caused by small-scale diffusion processes of solvents and gases into the molecular network of the co-polymer. Combining large scale molecular dynamics simulations and experiments, we address here the evolution of thermo-mechanical properties of shape memory polymers when they integrate small molecules by diffusion. Our results show that small molecules enhance the dynamics of structural relaxation and thus contribute to a softening of the material. Via a detailed analysis of the plastic activity and the elastic response, we provide evidence that the same effect is also responsible for increased plasticity and the gradual loss of the shape memory effect.

(I5 oral) **A FFT-based numerical homogenization tool for the study of the thermal expansion of a TATB-based pressed explosive**

H Trumel[1], J-B Gasnier[2], F Willot[2], D Jeulin[2], M Biessy[1] and E Laliere[1]

[1]CEA, DAM, Le Ripault, France, [2]MINES ParisTech, France

This presentation deals with a plastic-bonded explosive based on 1,3,5-triamino-2,4,6-trinitrobenzene (TATB), a triclinic energetic crystal. Pressing TATB powder mixed with a small amount of polymeric binder at high pressure yields a polycrystalline-like isotropic microstructure. The thermo-mechanical behaviour of the resulting material is fairly complex, displaying in particular dilatancy under thermal cycling, whose understanding is the aim of this study.

For this purpose, a numerical homogenization tool is being built. The microstructure is simulated by a locally anisotropic Johnson-Mehl three-dimensional tessellation model, identified to reproduce the measured grain size and elongation distributions. Grains are given random crystallographic orientations, from which local elastic and thermal expansion tensors are calculated from existing single crystal data. Periodic FFT-based thermo-elastic homogenization is performed on a 512^3 voxel virtual microstructure, yielding the three isotropic effective thermo-elastic moduli, compatible with existing theoretical bounds and with self-consistent predictions, and whose statistical accuracy is around 1%. Accounting for the binder yields only slight variations of effective moduli.

Predicted moduli compare favourably to experimental measurements performed under high superimposed pressure, but not to unconfined ones. This is attributed to the presence of micro-cracks, whose exploratory accounting will conclude the presentation.

(P1.44) **Megahertz frequency rheology of resin-filled silicone elastomers characterized by quartz crystal resonators**

J Yeh[1], R Schmidt[2] and K Shull[1]

[1]Northwestern University, USA, [2]Dow Corning, USA

With the continual widespread use of silicone elastomers, a thorough understanding of the mechanical properties of nano-sized resin filled silicones has become of academic and technological interest. These types of silicone material systems exhibit a range of dynamic mechanical heterogeneity, depending on the operational temperature and respective glass transition temperatures of the filler and matrix components. Although traditional dynamic mechanical tests can be performed, data analysis at high frequencies is difficult, due to the failure of the time temperature superposition principle. Also, interaction between the filler and matrix components can display an effective transition temperature, separate from the individual glass transition temperatures. In order to directly examine the viscoelastic properties at high frequencies, quartz crystal rheometers are utilized. This technique enables real time observation on the viscoelastic properties providing insight on the underlying mechanisms leading to changes in mechanical properties. A brief discussion on the physics of quartz crystal resonators and the viscoelastic model used to interpret the collected data will be provided. Also, the effects of operational temperature and filler loading in these silicone systems will be examined.

(P1.45) **Plastic events of polycrystals under cyclic deformation**

P Jana, M Alava and S Zapperi

Aalto University, Finland

Recently, Tamborini et al. have investigated plasticity of colloidal polycrystals, which are prepared by crystallizing thermo sensitive block copolymer Pluronics F108 with a small amount of nanoparticles as impurities, under cyclic shear. [1] Guided by their experiment, we perform plastic deformation study on 2D polycrystalline samples using molecular dynamics simulations. Samples are prepared by reducing the temperature of binary Lennard-Jones liquids with a fixed cooling rate. A small amount of bigger particles, which basically acts as an impurity, creates dislocations in the system because of size mismatch. A string of dislocations are defined as grain boundaries and the amount of impurities can control the number of grains. In the next stage, samples are undergone a cyclic deformation where the maximum strain amplitude (γ_{max}) is varied by changing the strain rate ((dγ/dt) (t)). For a small value of γ_{max}, the system becomes quiescent within a few cycles whereas for larger γ_{max}, particles move irreversibly which leads to the grain boundary motion and the annihilation of dislocations.

[1] Plasticity of a colloidal polycystal under cyclic shear. E. Tamborini, L. Cipelletti, and L. Ramos. PRL 113, 078301 (2014)

(P1.46) **Coarse-grained simulations of polymer matrix compites**

J El-Awady and A Aramoon

Johns Hopkins University, USA

In this talk we present a coarse-graining model for polymer matrix composites to characterize local properties and deformation at the matrix/fiber interface. In this coarse grained model the atomic structure is mapped to a set of coarse-grained particles that properly average the high frequency internal degrees of freedom of the molecule with all the conformationally relevant degrees of freedom taken into account. The derivation of coarse-grained potentials that include the conformational entropy of the system properly is achieved by using the intra-chain distribution function of the fully atomistic model at fixed temperatures. These temperature dependent coarse grained potentials were generated using electronic structure calculations, and incorporated into LAMMPS. A novel initialization cross-linking algorithm was also developed with topological constraints and is shown to develop polymer structures with up to 97% cross linked chains. The distribution of free volumes was predicted as a function of temperature and validated against available experiments. It is shown that the predicted free volume in a DGEBA-DAB matrix is in excellent agreement with experimental measurements. The current simulations also show a direct correlation between the free volume and the glass transition temperature. The simulations of the matrix/fiber interactions quantify the correlations between microstrucral variations (e.g. free volume, density, degree of cross-linking) with local mechanical properties as a function of position from the carbon fibers. Finally, the simulations characterize the bonding of matrix/fiber structure.

(P1.47) **Computational smart polymer design based on elastin protein mutability**

A Tarakanova[1], W Huang[2], D Kaplan[2] and M Buehler[1]

[1]Massachusetts Institute of Technology, USA, [2]Tufts University, USA

Soluble elastin-like peptides (ELPs) can be engineered into a range of physical forms, from hydrogels and scaffolds to fibers and artificial tissues, finding numerous applications in medicine and engineering as “smart polymers”. Elastin-like peptides are attractive candidates as a platform for novel biomaterial design as they exhibit a highly tunable response spectrum, with reversible phase transition capabilities. Here, we report the design of a library of elastin-like protein material models, using Replica Exchange Molecular Dynamics (REMD) methods for enhanced sampling, to study the effect of sequence identity, chain length, and salt concentration on ELPs’ structural transition, exposing molecular mechanisms associated with such modifications. This library is a valuable resource for recombinant protein design and synthesis as it elucidates effects and mechanisms at the single-molecule level, paving a feedback path between simulation and experiment for smart material design.

(P1.48) **Modelling of size effects in thin polymer films and characterization by molecular dynamics**

F Detrez and J Yvonnet

Université Paris Est, Laboratoire MSME, France

A multiscale model of thin polymeric films (see Figure 1) with size effects is constructed and characterized by molecular dynamics simulations. For this purpose, a continuum model including nonlocal elasticity is employed, whose elastic coefficients are identified by MD simulations on slab models of linear monodisperse polyethylene. Due to long-range effects in such materials, a procedure inspired from Yvonnet et al [1] is employed with different slab thickness to deduce the elastic coefficients. The continuum equations are solved by a FEM discretization and compared to the full MD model.

[1] J. Yvonnet, A. Mitrushchenkov, G. Chambaud and Q.-C. He. Finite element model of ionic nanowires with size-dependent mechanical properties determined by ab initio calculations. Computer Methods in applied Mechanics and Engineering, Vol. 200, pp. 614-625, (2011)

(P1.49) **The influence of crosslinking agents on the deformation mechanisms of thermosetting polymer: a molecular dynamics study**

H Park, B Kim, J Choi and M Cho

Seoul National University, South Korea

Deformation mechanism of amorphous polymer materials has been important but challenging issue for the engineering applications, since understanding the origins of elasto-plastic deformations require monitoring the complex molecular movements of polymer segments which is hard for experimental approach. Thus, in this study, the deformation mechanisms of epoxy polymer are investigated through the molecular dynamics (MD) simulations. Elasto-plastic material behaviour is characterized at the atomistic scale from the loading-unloading simulations. During the simulations, irreversible energy accommodations which imply the plastic behaviour of the epoxy chains is observed distinctly. The obtained result shows that the plastic deformation for the thermosetting polymer is mainly attributed to the non-bond interaction of the epoxy chains and the irreversible dihedral angle changes. Specifically, the dihedral angle types including the atoms of benzene rings in the model are easy to show the irreversible angle changes at the end of the loading and unloading simulations. Interestingly, these observations suggest the possibility of change of deformation energy accommodation and degree of plastic deformations with the different curing agents, since the redistribution of the deformation energy on the epoxy chains varies with the various structures of the hardner. Thus, we observe the local stress distribution of two prepared atomistic epoxy models during the deformations with same epoxy resin (diglycidyl ether of bisphenol A) and different curing agents (triethylenethetramine and diethylene toluene diamine), DGEBA/TETA and DGEBA/DETDA. This observation can help to understand the influence of molecular structure of the hardner on mechanical behaviour from the energetic and structural point of view.

(P1.50) **Multiscale approach to characterize crosslinking-dependent interphase region of epoxy nanocomposites**

B Kim, J Choi, H Shin and M Cho

Seoul National University, South Korea

In this work, we investigate the interphase region of epoxy nanocomposites using a multiscale approach combined with molecular dynamics simulations and a continuum regime. It has been well known that the reinforcing effect in nanocomposites is attributed to the formation of interphase in the vicinity of embedded nanoparticles. Herein, we focus on the crosslinking-dependent interphase characteristics in particular with regard to load transfer ability at the filler surface. Due to the complex communications at the filler surface with crosslinked epoxy molecules, a decisive conclusion has not yet been reached regarding the interfacial nature of crosslinked epoxy with fillers. In our previous work, we have revealed that the interfacial interactions are substantially disturbed by crosslinks among epoxy matrix. Since the interphase region is influenced by the variation of the interfacial attractive interactions, the fundamental characteristics of the interphase zone can be modified with the degree of crosslinking. As an extension of the previous work, starting from the effective interphase concept, the interphase behavior is studied on the basis of a mechanics-based multiscale scheme. For establishing the molecular models, spherical silicon carbaid nano-particulates are embedded into crosslinked epoxy matrix having different crosslink conversions. From the molecular models, local load transfer ability at the filler surface is examined in detail to determine the geometrical boundary of the interphase zone with incorporation of atomistic simulations and a continuum perspective. The internal mechanical behavior of interfacial region is further discussed considering the sophisticated dependency of the localized interphase zone in epoxy nanocomposites to crosslinking.

(P1.51) **Effective elastic properties of polymeric nanocomposites including the cluster of nanoparticles: Multiscale homogenization approach**

M Cho, H Shin, J Han and J Choi

Seoul National University, South Korea

In this study, a multiscale modelling strategy of polymeric nanocomposites including the clustered nanoparticles is proposed. To reflect interface effect that stems from highly condensed polymer near the nanoparticle, effective interphase zone is introduced as a single phase with finite thickness. As filler agglomeration is processed, interphase zone of the clustered nanoparticles are percolated. An influence of interphase percolation on the homogenized elastic properties of nanocomposites is obtained from molecular dynamics simulation quantitatively. As inter-particulate distance decreases less than 2nm, the degradation of homogenized elastic properties is investigated remarkably. Through the multiscale bridging method with finite element homogenization, interphase elastic properties with respect to the overlapped density, the volume of overlapped interphase zone over that of total interphase zone, are inversely obtained. It is clearly verified that overlapped interphase model is applicable to the homogenization of multi-particulate system. To investigate an influence of cluster size on the homogenized elastic properties of polymer nanocomposites, multiscale homogenization analysis is conducted for various cluster size, described by the number of clustered particles. The cluster includes the 1, 4, 10, and 30 numbers of particles at fixed radius and volume fraction of nanoparticles as 3% and 9Å, respectively. Simulation results show that the homogenization results clearly declined as the cluster size increases. In future work, a multiscale modeling framework to obtain the effective elastic properties of cluster with propose of inverse analytic algorithm.

(P1.52) **Flow induced alignment of dilute collagen acidic solutions in simple shear and mixed shear-extensional flows for biological plywood formation**

O Gutierrez and A Rey

McGill University, Canada

The dynamic behaviour of natural structural compounds solutions is of great interest for creating biomimetic materials, tissue engineering purposes, among other applications since they are widely used in non-equilibrium self-assembly processes to create the so-called biological plywoods whose building blocks are arranged with a helical axis resembling chiral nematic liquid crystalline phases. These processes make use of coating flows of biopolymer solutions where the macromolecules are submitted to shear and extensional deformations to dynamically align the respective building block for later evaporation processes to create the aforementioned materials. This work focuses on the theoretical rheological study of collagen acidic solutions with applications towards collagen films presenting no defects only if the time-scales associated to the structure relaxation, helix formation and evaporation rate are well synchronised. The study was carried out in two parts: i) Simple shear flow configuration which allowed a physical parameter estimation through simulations that were validated with previously reported experimental data and ii) Four-roll mill configuration with mixed kinematics (shear and extensional deformations) allowing to analyse the role a kinematic parameter to the alignment and ordering of the collagen molecules and estimate the value required in the process given the drying conditions.

(P1.53) **Nanocavitation during deformation of PE/CNT nanocomposite**

N Orekhov and V Stegailov

Joint Institute for High Temperatures of Russian Academy of Sciences, Russia

In the present work, the structural properties of a polyethylene (PE) matrix in contact with carbon nanotubes (CNT) during deformation are studied via the classical all-atom and coarse-grained molecular-dynamics methods.

CNTs have proved to be very promising fillers for polymer nanocomposites, allowing to affect its mechanical properties significantly even at small concentrations (on the order of several weight percent or even less). However, there is still no clear understanding of the principles of the nanoinclusion interaction with polymer matrices and the nature of its strengthening on the molecular level. The properties of polymer chains in contact with a nanoscale filler surface inevitably differ from the properties of a pure polymer. Because of the large area of their effective surface, even at small concentrations of nanoinclusions, the interfacial area may cover a substantial volume of the polymer matrix, i.e. large part of polymer chains contact with nanoparticles. Thus, the dynamics of nanovoid nucleation in nanocomposite during deformation differs from the case of pure polymer. Extending our previous results on the CNT geometry correlation with the elastic properties of PE/CNT nanocomposite [1], we investigate here the influence of nanoinclusions with high aspect ratio on the entanglement network in polymer nanocomposite, the process of disentanglement during deformation and dynamics of subsequent nanovoid nucleation.

The work was supported by the Russian Science Foundation (Grant No. 14-50-00124).

[1] N.D. Orekhov, V.V. Stegailov "Simulation of the Adhesion Properties of the Polyethylene/Carbon Nanotube Interface", Polym. Sci., Ser. A 58 (3), 476 (2016)

(P1.54) **Comparative study of two anisotropic damage models based on multi-mechanisms approaches for semi-crystalline polymers**

W Ayadi[1], L Laiarinandrasana[2] and K Sai[3]

[1]Institut Supérieur des Etudes Technologiques de RADES, France, [2]MINES ParisTech, Centre des Matériaux, France, [3]Ecole Nationale d'Ingénieurs de Sfax, France

In this work, a comparative study between Continuum Damage Mechanics (CDM) and Porous plasticity (PP) approach is performed in order to modelize the anisotropic damage behavior of semi-crystalline polymers (SCPs). Both models are related to the Multi-Mechanism (MM) approach in which a first mechanism is assigned to the amorphous phase and a second mechanism to the crystalline phase. The constitutive equations are developed within thermodynamic framework and take into account the degree of crystallinity of the SCP. This comparison is based upon tensile tests for large deformation history conducted on notched round bars specimen (NRBS) made of Polyamide 6 (PA6) to enhance a triaxiality stress state. For CDM model, the anisotropic damage is described using a tensorial variable based on the net stress concept whereas the microstructure morphology of the cavities was considered for the PP model. The anisotropic damage is controlled using a shape factor parameter defined as the ratio between the void diameter and the void height. It is found that both CDM and PP approach coupled with MM model are successful in predicting the anisotropic induced damage of the SCP at different stage of a large deformation history. Moreover the PP model damage is more relevant in predicting the microstructural morphology of the voids at a real scale.

Symposium J

(J1 invited) **Shear-coupled grain boundary motion: Atomistics to continuum**

Y Mishin

George Mason University, USA

Recent experimental research and atomistic modeling have led to the recognition that many grain boundaries (GBs) in crystalline materials can couple to applied shear stresses and be moved by them in a manner similar to dislocation glide. During this “coupled” GB motion, the boundary produces shear deformation of the lattice it traverses and causes relative translation of the grains. For curved GBs, the coupled GB motion creates a driving force for grain rotation. These coupled processes can lead to interesting phenomena in polycrystalline, and especially nanocrystalline materials, such as stress-induced grain growth and stress-induced grain rotation. This talk will present an overview of the current knowledge of the shear-coupling effect based from experiments and recent simulations by molecular dynamic (MD) and other methods. On the continuum side, application of irreversible thermodynamics allows one to derive the driving forces and phenomenological equations for a number of processes occurring at a moving GB, such as generation and annihilation of new sites, normal motion, sliding and grain rotation. The shear-coupling effect is introduced into the theory by imposing certain geometric constraints on GB motion and grain translations. These constraints, in turn, modify the driving force for GB migration and other processes. Possible couplings between the atomistic and continuum descriptions of GB motion are discussed.

(J1 oral) **Atomistic migration mechanisms of grain boundaries deviated from the symmetric tilt orientation**

S Hadian[1], B Grabowski[1], C Race[2] and J Neugebauer[2]

Max-Planck-Institute, Germany

We have studied the kinetics and atomistic mechanisms of migration in grain boundaries with general mixed planes in the vicinity of a symmetric tilt <111> Σ7 grain boundary in aluminium. Using physically converged simulations and investigating migration snapshots in 3D, we find unique characteristic mechanisms in the motion of non-symmetric grain boundaries as compared with the symmetric one. The mixed grain boundaries show nano-faceting which enables two heterogeneous atomistic migration mechanisms that are fundamentally different from the previously reported homogeneous defect nucleation mechanism in the symmetric tilt boundaries: Depending on the orientation of the nano-facets/steps either a double kink nucleation and propagation or a pure kink flow drives the motion. We show that these atomistic mechanisms are the origin of the observed change from a strongly non-Arrhenius behavior towards a linear Arrhenius behavior, and of the change in the asymptotic behavior of the migration barrier at low driving forces.

(J1 oral) **Examining the interplay of tension and shear for a metal grain boundary through atomistic ab initio computational studies**

F Ehlers, S Queyreau, M Seydou, D Tingaud, Y Charles and F Maurel

Université Paris Diderot, France

For efficient integration in a multiscale modeling scheme, atomistic supercell based studies of grain boundaries (GBs) with first principles methods must address a mixed mode loading process. In spite of the abundance of examples from larger scale modeling as well as experiment stressing the evident need of such simulations, close to all density functional theory (DFT) based studies of GBs still focus on the simpler loading mode of unaxial tensile strain. As a consequence, general trends for the GB response to realistic loading processes largely remain unknown. Probing the influence of combined tension and shear on the structure and energy of a selected Al GB in DFT based computational studies, we highlight and discuss the presence and importance of such trends, stressing an unexpected interplay between the two fundamental components of the loading mode.

(J1 oral) **Effect of a normal stress on the shear-coupled grain boundary migration**

N Combe, F Mompiou and M Legros

Cemes, CNRS UPR 8011 and Universite de Toulouse, France

Grain boundary (GB) migration occurs in stressed nanocrystalline materials (grains sizes <100 nm) as an alternative vector of plasticity compared to the usual dislocation activity. The shear-coupled GB migration, the expected most efficient GB based mechanism, couples the GB motion to an applied shear stress [1,2]. Stresses on GB in polycrystalline material have however seldom a unique pure shear component.

The influence of a normal stress on the shear coupled GB migration is investigated in a copper bicrystal studying the Σ13 (320) GB. Using molecular dynamic simulation, we theoretically show that the yield shear stress inducing the GB migration strongly depends on the applied normal stress. Moreover, we show that the application of a normal stress may induce a modification of the observed GB migration mechanism (mode). We evidence the existence of the $[010]$ GB migration mode, theoretically predicted but never observed. We characterize this mode both structurally and energetically using the nudeg elastic band method.

[1] Rajabzadeh, A.; Mompiou, F.; Legros, M. and Combe, N. Phys. Rev. Lett., 110, 265507 (2013)
[2] Combe N.; Mompiou, F.; Legros, M. Phys. Rev. B, 93, 024109 (2016)

(J2 invited) **From random-walk to stress-driven grain boundary motion in pure FCC metals**

C Brandl

Karlsruhe Institute of Technology, Germany

The motion of grain boundaries (GBs) is crucial for the evolution of microstructure both in processing and in application. In experiments, the grain boundary motion is usually studied at relatively high homologous temperature during long times under small mechanical loads. But grain boundary motion is also shown to be a deformation mechanism occurring at high stresses and relative low temperatures, as for example in deformation studies of nanocrystalline metals and shock loading.

Using molecular dynamics (MD) simulations, the GB motion is used to elucidate the role of atomistic structure (morphology) and velocity-driving force relation (mobility) for two different driving force mechanisms: elastic anisotropy (asymmetric S3 GB) and shear coupled motion (symmetric S11). As function of temperature and driving force, the GB mobilities show for both GBs a complex nonlinear behavior beyond the conventional conjecture of Arrhenius-like temperature-dependence in mobility and linear velocity-driving force relation by the motion of the same constituent GB defects.

The low driving force limit is investigated by analyzing the random-walk and fluctuations of the GB at zero driving forces utilizing the temperature-accelerated dynamics for the motion below the roughening transition temperature. The mechanisms are compared to the finite driving-force motion and its implications on the GB mobility are discussed.

The observed dynamics regimes – with and without driving-force - are compared to a novel phenomenological mesoscale model, which shows the similar range of the observed mobility regimes; and which also accounts for the hierarchic nature of the GB motion as e.g. GB kink-formation and GB kink-drift.

(J2 oral) **Atomistic shear deformation mechanisms of interfaces in TiAl**

R Janisch, M Kanani and A Hartmaier

ICAMS, Ruhr-Universität Bochum, Germany

Interfaces in metallic micro- and nanostructures play a role during plastic deformation in many respects. Besides accomodating part of the plastic strain by means of grain boundary sliding and migration they can act as sources, sinks, or barriers for dislocations, as well as as crack nucleation sites. These processes are not independent, and often several of them occur at the same time. Since they are determined by details of the atomistic structure and interatomic bonding it is challenging to derive any constitutive relationships that are transferrable to different interface types and loading conditions. However, in this work we were able to relate the observed mechanisms at interfaces in γ-TiAl to structural features of the grain boundaries and their generalized stacking fault energy (GSFE) surfaces, thus providing the foundation for such a description.

To isolate the intrinsic deformation mechanisms of the interfaces molecular statics and molecular dynamics simulations of bicrystal shear were carried out for different rotational boundaries in γ-TiAl. Four distinct mechanisms could be identified, namely rigid grain sliding, grain boundary migration, coupled sliding and migration, and dislocation nucleation and emission. Depending on the loading direction different mechanisms can occur at one and the same grain boundary, i.e. there is a pronounced anisotropy in the interfacial shear behaviour. This anisotropy is suggested as the explanation for seemingly contradicting experimental results in the literature and it is reflected in the GSFEs of the interfaces. An extended multilayer-analysis of these GSFEs allows to relate the observed atomistic mechanism to their basic features.

(J2 oral) **Modelling plastic deformation in interface dominated microstructures using a dislocation based continuum formulation**

M Sudmanns, K Schulz, S Schmitt and P Gumbsch

Karlsruhe Institute of Technology, Germany

The striving for advanced materials with well-defined microstructures has led to an increasing effort towards a physically based description of the motion of dislocations as the cause of plastic deformation and the origin of materials failure. Several dislocation based continuum theories have been introduced, but only recently rigorous techniques have been developed for performing meaningful averages over systems of moving, curved dislocations, yielding evolution equations for a dislocation density tensor.

Regarding a self-consistent coarsening of dislocation modelling in order to construct an efficient numerical implementation, several issues have to be solved including calculation of the stress field of a system of dislocations, correlation functions, and boundary conditions. Accurate solutions have been found for one dimensional systems. The understanding and development of predictive modelling techniques for determining the influence of interfaces on the overall response of a material is a central aspect for the design of new materials and the optimization of currently used materials.

In this presentation, we discuss the role of internal interfaces in a continuum representation of dislocation microstructures for fully two- and three-dimensional systems. We consider the dislocation interaction across grain boundaries for different orientation of the slip systems as well as simplified composite materials. The results are compared to ensemble averages over discrete dislocation distributions, leading to a more physical continuum approach of dislocation interactions close to internal interfaces.

(J2 oral) **Effects of interfaces on deformation mechanisms and their optimization in TiAl intermetallic alloys**

D Xu[1], C Teng[1], HWang[1], Y Wang[2] and R Yang[1]

[1]Chinese Academy of Sciences, China, [2]Ohio State University, USA

TiAl-based alloys in replacement of Ni-base superalloys as low pressure turbine enhance greatly the performance of aero-engines. However it is still challenging to meet the requirements for certain mechanical properties and long term stability. It is recognized that the dual-phase lamellar structure, although still being relatively brittle, has the best balanced mechanical properties. Extensive efforts have been made in recent years to understand how the various interfaces affect the deformation mechanism and how to control the lamellar structure to achieve improved properties. In parallel to experimental efforts, multiscale simulations have been carried out to understand the mechanisms of deformation and microstructure evolution. For example, our energetic calculations and MD simulations show that, among the four types of lamellar interfaces, the twin boundary has the lowest energy and is most stable against deformation and, thus, should be beneficial for long term stability of the alloy working at elevated temperatures. On the other hand, our phase field simulations show how variations in interfacial energy, elastic energy, phase transformation driving force and external stress affect the fraction of twin interfaces during microstructure formation, shedding some light on how to design heat treatment routes to maximize the twin boundary fraction.

(J3 invited) **Atomistic study of mechanism transition of grain boundary motion and dislocation nucleation from grain boundary**

S Ogata and J-P Du

Osaka University, Japan

Grain boundary motion and dislocation nucleation from grain boundary are key plastic deformation units of ultra-fine grained metals because of the less intra-grain dislocation sources and activities in the nano-sized grains. Since these plastic deformation units are atomistic scale and consist of thermally-activated processes at finite temperature, a dynamic atomistic simulation, like molecular dynamics (MD) simulation, is only the way to figure out the details. However, these thermally-activated processes are usually very rare-events from the viewpoint of the typical time-scale of the atomistic simulation. Thus a longer time-scale coarse-grained atomistic simulation method is necessary to analyze these processes. Recently, we have developed an accelerated MD simulation method that is called adaptive boost MD method. In this study, we applied this method to investigate them and eventually figured out mechanism map of these events with respect to applied temperature and stress. We found mechanism transition from displcacive to diffusive in grain boundary motion and from single to multiple dislocation nucleation in the dislocation nucleation from grain boundary.

(J3 oral) **Influence of hydrogen on grain boundary cohesion in nickel**

M Mrovec[1], D Di Stefano[2], B Ziebarth[2] and C Elsässer[2]

[1]ICAMS, Ruhr University Bochum, Germany, [2]Fraunhofer IWM, Germany

The presence of hydrogen in metals often leads to marked lowering of their ductility, fracture strength and fracture toughness – a phenomenon commonly known as hydrogen embrittlement (HE). One of possible HE mechanisms is related to segregation of hydrogen at grain boundaries (GBs) that weakens the GB strength and results in easier intergranular decohesion. It has been observed that the susceptibility to hydrogen-induced intergranular embrittlement varies for different microstructures and hydrogen concentrations. However, quantitative knowledge of key quantities such as hydrogen binding energies at various GBs or critical hydrogen concentrations for fracture is still limited.

In this theoretical study, we explore the interaction of H with several grain boundaries in Ni at the atomic scale using first principles calculations based on density functional theory (DFT). We calculate H diffusion barriers and segregation energies in the vicinity of the GBs and relate these quantities to the geometrical characteristics of structural units composing the GBs. In addition, we also investigate the influence of H concentration on the cohesive behavior of the investigated GBs and compare the theoretical predictions with existing experimental results.

(J3 oral) **Strength of interfaces with segregated impurities from first principles**

M Cerny, P Sestak, P Rehak, M Vsianska and M Sob

Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Czech Republic

In our first-principles study, we calculate the ideal strength of coherent interfaces and symmetrical grain boundaries (GB) under uniaxial tension applied perpendicularly to the interface. Computational supercells are subjected to three different modes of simulated deformation comprising shift of rigid grains, uniaxial deformation with optimized atomic coordinates and fully optimized uniaxial loading. The results are mutually compared and the effect of segregated impurities on the tensile strength is discussed. The comparison reveals not only the effect of the impurities on the ideal strength but also the importance of full lattice optimization during the simulation of tensile test.

(J3 oral) **Hydrogen induced grain boundary decohesion in Nickel extracted from Molecular Dynamics Simulations**

D Spearot[1] and R Dingreville[2]

[1]University of Florida, USA, [2]Sandia National Labs, USA

The influence of hydrogen on intergranular fracture in Ni during steady-state crack propagation is studied via molecular dynamics simulations. Rather than using a traditional angle/axis approach to select grain boundaries, sets of bicrystal interfaces are selected in this work via a mechanics-based approach designed to isolate the inherent strength of the grain boundary from the properties of the neighboring lattices. Equilibrium hydrogen coverages and favorable sites for hydrogen segregation are motivated by Monte Carlo calculations for select misorientations. Decohesion behavior is quantified through extraction of a traction-separation relationship during steady-state crack propagation, with the aim of producing data that can be used in higher-length scale simulations of predictive fracture. A sensitivity analysis is performed on the CZVE approach, clarifying the role of CZVE size and numerical parameters necessary to differentiate elastic and decohesion data. For a <110> Σ3 {112} symmetric tilt grain boundary, results show that increasing hydrogen coverage leads to a general decrease in the work of separation and promotes a reduction in the peak stress in the extracted traction-separation relationships.

(J3 oral) **Hydrogen segregation to grain boundaries in nickel**

R Dingreville[1], C O'Brien[1], S Foiles[1] and S Berbenni[2]

[1]Sandia National Laboratories, USA, [2]UMR CNRS 7239, Universite de Lorraine, France

Solute-atom segregation to grain boundaries substantially affects their fundamental physico-chemical properties, which in turn impacts a wide range of material behaviors. The chemical equilibrium distribution of solutes in a solid determines the interaction between these solutes and defects already existing in a material system and plays a key role in the nature of the subsequent mechanisms governing their mechanical behavior.

In this presentation, we consider hydrogen segregation to grain boundaries by modeling solute atoms as misfitting inclusions within a disclination structural unit model describing the grain boundary structure and its intrinsic stress field. The solute distribution around grain boundaries is described through Fermi-Dirac statistics of site occupancy.

The susceptibility of hydrogen segregation to symmetric tilt grain boundaries in nickel is discussed in terms of the misorientation angle, the defect type characteristics at the grain boundary, temperature, and the prescribed bulk hydrogen fraction of occupied sites. This continuum construct is compared to an atomistic model of the same grain boundaries by using a grand canonical Monte Carlo technique to determine the degree of hydrogen segregation. For certain grain boundaries, due to the complex interaction of the boundary structure and segregation mechanism, limitations of the model will be discussed.

Segregation susceptibility over a wide range of grain boundary characters typical of those observed in polycrystalline materials will be ascertainedin the context of grain boundary engineering. Such simplistic continuum theoretical tool can be used to orient specific experiments or corresponding atomistic simulations.

(J4 invited) **Effect of bi-phase interfaces on texture evolution in HCP/BCC nanolaminates fabricated by severe plastic deformation**

I Beyerlein

University of California at Santa Barbara, USA

Over the years, two-phase nanolaminate thin film composites have demonstrated an unusually broad number of desirable properties, such as high strength, high strain to failure, thermal stability, and resistance to light-ion radiation. Recently we have shown that bi-phase HCP/BCC nanolaminates with layer thicknesses < 50 nm can be made via severe plastic deformation (SPD) in bulk sizes suitable for structural applications. Mechanical testing of these HCP/BCC nanolaminates shows exceptionally high strength and characterization via a suite of techniques indicates that the crystals are highly oriented. While the cause of these unusual properties can easily be associated with a high density of bimetal interfaces, how the interfaces physically control microstructural evolution and macroscopic properties remains an area of intense research. This presentation highlights our modeling and experimental efforts to understand and link the evolution of the nanostructure, the interface properties, and preferred texture during the SPD process.

(J4 oral) **Multi-scale simulation of mechanical properties of carbide-metal interfaces from first-principles calculations**

E Barbé, C C Fu and M Sauzay

CEA Saclay DEN/DMN/SRMP, France

Fracture of interfaces between some carbides and a metallic matrix is often observed during creep. Such fracture may be responsible for the interfacial creep cavitation and ductile damage. Understanding the mechanisms of fracture allows to predict the creep lifetime and ductile damage evolution. This study focuses firstly on coherent interface between a metallic matrix (Fe, Cr, Ni) and a representative carbide, Cr23C6.

Formation energy of free surfaces and interfaces are calculated by a method based on analysis of chemical potentials. The energy of fracture as defined by the Griffith's energy is deduced from these values. Then, interfacial fracture stresses can be estimated by the UBER model (universal energy bonding relationship (Rose & al (1981), Rice & al (1989)), where the physical ingredients (interfacial thickness, Young's modulus of interface and fracture energy) are calculated based on Density Functional Theory. We consider metallic systems with different chemical composition, crystallographic structure and magnetic ordering, in order to investigate the dependence of the mechanical behavior on these properties. We predict that coherent interfaces show rather high fracture stresses, which is compatible with recent experimental observations showing that the interfacial fracture rather occurs at incoherent interfaces. Therefore, we also address some most relevant semi-coherent interfaces and investigate the effect of impurity (P, S) segregation.

(J4 oral) **'Elastic-perfect plastic' behavior in elongated Au-Si core-shell nanowires due to the confinement of the dislocations by a hard amorphous shell**

J Godet[1], C Furgeaud[1], L Pizzagalli[1] and M J Demkowicz[2]

[1]Pprime Institute University of Poitiers, France, [2]Texas A&M University, CUSA

In order to evaluate the role of a hard amorphous silicon (a-Si) shell on the deformation of a soft crystalline gold core, we have investigated the mechanical properties of the Au@a-Si core-shell nanowire (NW) by molecular dynamics simulations. We have first optimized an existing parametrization of the MEAM potential to better reproduce the mechanical properties of gold and silicon as well as the Au-Si interactions. The comparison of the tensile tests performed on pristine Au NW, a-Si shell and Au@a-Si core-shell NW reveals that the hard amorphous shell works against the growth of ledges left by localized plasticity. In consequence, the localized plasticity and the expansion of nano-twin are reduced. The confinement of the dislocations in the core due to the hard shell do not lead to an apparent hardening of the nanostructure. But a homogeneous plastic deformation of the core-shell nanowire is observed at almost a constant flow stress equal to the yield stress. This behavior is characteristic of an elastic-perfect plastic material.

(J4 oral) **Multiscale modeling of heterophase interfaces between alpha zirconium and gamma-ZrH hydrides**

R Besson, M-A Louchez, L Thuinet and A Legris

UMET, France

We present a joint atomic-scale and mesoscale investigation of heterophase interfaces between gamma-ZrH hydrides and hexagonal alpha zirconium. Basal interfaces were modelled using multilayered alpha|gamma systems with various periods and phase proportions in ab initio calculations, a convenient way to separate out coherent interface energies from elastic contributions. As a particular interest, our approach allows to describe the influence of local hydrogen composition on coherent interfaces, namely the interactions between long-range elastic effects and chemistry. In the case of prismatic interfaces, the different stacking sequences in both phases (ABC for gamma hydrides and AB for alpha Zr) were found unstable for the small systems tractable from ab initio calculations, and prismatic alpha|gamma interfaces were thus studied in a continuous framework. The geometrical accommodation of both phases being achieved through the introduction of networks of dislocations in the prismatic planes, these dislocations were relaxed within an extended Peierls-Nabarro model relying on hybrid generalized stacking faults obtained from ab initio calculations. Our work allows to feed phase-field precipitation models with correct interfacial energies. It also provides new insights into the currently controversial interpretations of experimental results on hydride preferential habit planes.

(J5 invited) **Chemo-thermo-mechanical framework for the prediction of stress evolution during metal oxidation**

A Benzerga[1], A Roos[2], P Kanoute[3] and J-L Chaboche[3]

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Thermal protection systems are commonly used in power generation plants and engines to limit heat transfer to key components and protect constituent materials from oxidation and hot corrosion. Stress evolution in this multilayered system plays a key role in driving damage and failure mechanisms. Yet, its modeling is still based on oversimplifying assumptions about the constitutive behavior of the metallic and oxide layers, which often fall in the micron or sub-micron range. Here, we tackle the simpler problem of an oxidation couple and aim at computing stress evolution in both layers concurrent with oxidation. Oxide thickening is modeled using widely adopted phenomenology but stress evolution is affected by the diffusion of cationic and anionic vacancies in the polycrystalline oxide layer while treating the metallic layer as either (i) elastic or (ii) elastic-plastic with plasticity described using discrete dislocations. In the oxide, grains are modeled as columnar and grain boundaries act as fast diffusion pathways mediating matter transport that accompany further oxide thickening. A computational framework for solving problems of dislocation-mediated creep coupled with point-defect diffusion is presented. Time scale separation is contingent upon the existence of quasi-equilibrium dislocation configurations. A variational principle is used to derive the coupled governing equations for charged point-defect diffusion and dislocation climb along grain boundaries.

(J5 oral) **Phase field modelling of growth and failure of oxide intrusions along grain boundaries**

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The development of oxide intrusions along grain boundaries is observed prior to intergranular stress corrosion cracking, which is why they have been naturally suspected to be the starting point of such cracks. Nevertheless, the underlying crack nucleation mechanism remains unclear, which constitutes an obstacle to the accurate estimation of stress corrosion cracking. The nuclear industry, amongst others, has shown a great interest in solving such a problem to optimise its productivity while ensuring high safety requirements. In this work, evidences of the self-weakening role of intergranular oxide penetrations leading to the nucleation of surface cracks are shown on the basis of phase field calculations.

A modelling framework has been developed accounting for a generic ternary two phase system coupled with separate mechanical behaviours up to damage. The framework couples multicomponent diffusion and strains, which is decomposed into four contributions, where damage and transformations strains are considered alongside the classical elastic and plastic parts. To that, the framework is coupled with additional grain boundary fields accounting for anisotropic grain boundary diffusion and brittle failure.

Finite element simulations are performed (i) 1D simulations highlight the role of mechanical loads on the breakaway oxidation kinetics (ii) 2D simulations of growing oxide intrusions reveal the delayed and progressive generation of tensile tractions at the free surface along with the influence of creep loads. Such a first insight on the early stage of intergranular stress corrosion cracking is finally discussed.

(J5 oral) **Material parameter identification by using atomistic-to-continuum homogenization for thermo-mechanically coupled problems**

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The atomistic structure defines the thermo-mechanical response of any material on the continuum scale. Within this talk, a general homogenization framework for the atomistic-to-continuum transition of thermo-mechanically coupled materials is presented. For that purpose, molecular dynamics simulations are coupled with continuum mechanics simulations by means of the principle of energy equivalence. Numerically, a Ritz-type approximation of this infinite dimensional problem is elaborated. In contrast to other existing approaches (e.g. Universal Energy Binding Relationship), full relaxation, i.e. equilibrium, on both scales is guaranteed (molecular and continuum). Furthermore, since the approach is based on the total energies of the representative volume elements, localized quantities, such as local energies or stresses and strains are not required. For this reason, the advocated homogenization approach can also be employed for a density functional theory to continuum transfer. However, this type of transfer is not considered in the talk.

(J5 oral) **A thermodynamically consistent diffuse interface crystal plasticity model to study grain growth during dynamic recrystallization**

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Dynamic recrystallization can be defined as a spontaneous change in the microstructure of a deformed crystal during deformation at an elevated temperature due to the growth of defect-free grains through the motion of high angle grain boundaries. Grain growth in a polycrystalline material occurs due to the combined effect of grain rotation and the motion of grain boundaries to minimize surface area. Grain evolution, in the absence of stress, is commonly modeled using the Kobayashi--Warren--Carter (KWC) model, a phenomenological model developed by Kobayashi et al. [1998]. In the presence of stress, grain evolution is a result of interplay between bulk and grain boundary dislocations. In this work, we study the phenomenon of dynamic recrystallization in bcc tungsten using a diffuse interface crystal plasticity model. This model generalizes the existing KWC model using kinematically derived evolution laws for bulk and grain boundary dislocations. The constitutive law of the model is expressed in the form of grain boundary free energy function of grain boundary dislocation content, and bulk free energy function of the Lagrangian strain and bulk dislocation content. Therefore, obtaining grain boundary and bulk free energies, and grain boundary mobilities from an atomistic simulation results in a multiscale model. Moreover, the model is derived within a thermodynamically consistent framework, and accounts for non-uniform temperatures.

[1] Kobayashi, Warren, and Carter. Vector-valued phase field model for crystallization and grain boundary formation. 119:415–423, 1998.

(J5 oral) **Collective influence of texture, grain shape, size and dislocation density on the plasticity of polycrystalline metallic thin films**

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Freestanding metallic thin films often show a sharp crystallographic texture and columnar nanosized grains with mostly one grain along the thickness [1]. Enhanced strength and fatigue resistance of such nanocrystalline thin films are often accompanied by a lack of ductility. However, recently, moderate to high ductility of thin films has been reported [2]. This raises some fundamental questions about the active deformation mechanims and also the modeling using classical dislocation based hardening approach.

In this paper, we report the collective influence of texture, grain shape, grain size and dislocation density distribution on strain hardening behavior; and on the transition from dislocation based to grain boundary nucleation based hardening. Thereby, providing some insight into the experimentally measured high ductility. Firstly, we perform three dimensional discrete dislocation dynamics simulations on individual grain of same volume but different aspect ratios to understand how the grain shape influences slip system activity. Then, the polycrystalline version of the dislocation dynamics code, TRIDIS coupled with a finite element methods [3], is used to perform simulations of a film multi-crystal. Results reveal the importance of grain size and dislocation density distribution on strain hardening of metallic thin films.

[1] W. D. Nix, Elastic and plastic properties of thin films on substrates, MSEA, 234-236, 37-44 (1997)
[2] M. -S. Colla et al., High strength-ductility of thin nanocrystalline palladium films with nanoscale twins, Acta Mater., 60, 1795-1808 (2012)
[3] M. C. Fivel and G. R. Canova, Developing rigorous boundary condition to simulations of discrete dislocation dynamics, MSMSE, 5-7, 753 (1999)

(J6 invited) **large scale atomistic simulations of the interaction of single arm sources with grain boundaries in FCC bipillars**

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Large scale 3D atomistic simulations are used to study the interaction of single arm sources with grain boundaries in Ni and Cu bipillars. Both a large angle grain boundary and a low angle twin boundary are considered. It is shown that a large angle boundary is a strong obstacle to dislocation source operation whereas the single arm source overcomes the low angle twin boundary at low stresses by cross-slip. It is suggested that large-scale 3D atomistic simulations are required to properly understand these interactions. These atomistic simulation results are used to explain the experimental mechanical behavior data on Cu bipillars with a similar large angle grain boundary or a twin boundary.

(J6 oral) **Critical intergranular porosity for a transition from intrinsinc ductility to brittleness**

D Tanguy

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Crack propagation along the S 33 (554)[110] symmetrical GB, in the presence of an increasing density of nanoscale cavities, is simulated by Molecular Statics. The crystallography is such that straight dislocations can be easily emitted at the crack tip. Cavities are found to increase the critical stress intensity factor by up to a factor two. Nevertheless, emission and twinning still occur at the expense of crack propagation. To overcome "lattice trapping", specific equations of motion are used to constrain Shockley partial emission: the tip is rendered brittle. After propagation is initiated, the constraint is switched off and the ability of the damaged GB to resist cracking can be properly evaluated. One void configuration is found to truly cause brittle fracture. By comparison to the others, a critical porosity is found. Furthermore, the stress field along the GB is calculated from the distribution of the infinitesimal dislocations along the crack plane. It enables to extract the traction-separation relation from the atomistic data and calculate the work of separation Wsep (constrained cracks are used for the ductile configurations). Values range from 3 to 5.5 J/m2 (three times the ideal work of fracture). Surprisingly, the brittle configuration does not have the lower Wsep, which contradicts the simple idea that embrittlement is due to a drop of Wsep. A close look at the mechanisms shows that the initiation of void growth is necessary to smooth the opening profile and switch off dislocation emission while Wsep also depends on the thinning of bridges.

(J6 oral) **Atomic scale study of twinning in Zirconium**

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Plasticity in zirconium, as well as in many other hexagonal close-packed metals, is controlled by the glide of dislocations with <a> Burgers vectors. Those dislocations can however not explain any deformation along the <c> axis and at low temperatures twinning is activated to accommodate such a strain. In this work, we focus on the mechanisms controlling twin growth using atomistic simulations relying either on an empirical interatomic potential of the EAM type or on ab initio calculations. The four different twinning systems, which can be activated in zirconium depending on the temperature or the applied strain, are modeled. We first study the perfect twin boundaries showing the ability of the EAM potential to predict their structures and relative energies taking the ab initio calculations as a reference. We then focus on the disconnections, i.e. the twinning dislocations which are responsible of the twin growth. For a given twinning system, several disconnections of different Burgers vectors, different heights and different core structures exist. Considering all these disconnections, we calculate their formation and migration energies using the NEB method. The elastic interactions between the defects and their periodic images are computed using linear inhomogeneous anisotropic elasticity, allowing to extract disconnection core energies that are intrinsic properties of the disconnections, independent of the cell dimensions. We use this information to develop a kinetic model of twin growth and study the competition between the different growth modes under various stress states.

(J6 oral) **The role of interfaces in nucleation of dynamic damage in FCC and BCC materials**

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Los Alamos National Laboratory, USA

For ductile metals, the process of dynamic fracture occurs through nucleation, growth and coalescence of voids. For high purity single-phase metals, it has been observed by numerous investigators that voids tend to heterogeneously nucleate at grain boundaries and all grain boundaries are not equally susceptible to void nucleation. Several factors can affect the failure stress of a grain boundary, such as grain boundary structure, energy and excess volume, in addition to its interactions with dislocations. Flyer plate simulations were carried out for four boundary types with different energies and excess volumes in both materials. These boundaries were chosen as model systems to represent various boundaries observed in “real” materials. In this work, we will compare the mechanisms behind void nucleation in FCC (Cu) and BCC (Ta) materials by using molecular-dynamics simulations. We will also explore the influence of grain boundary energy, excess volume and plasticity at the boundary on the failure stress of a grain boundary.

(J7 invited) **Boundary layer formation in continuum dislocation dynamics**

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A comparative study between discrete and continuum dislocation dynamics (DDD and CDD) for the analytically tractable case of a circular plastic inclusion of varying size within an elastic medium is carried out in two dimensions under single slip conditions. The CDD formulation distinguishes signed edge and screw dislocation types [1], explicitly treats formation and destruction of dislocation dipoles, and considers the dislocation flux in the (non-) local density evolution. The continuum model matches the discrete dislocation dynamics results to a large extent. Mesh-dependent density oscillations develop in CDD due to an instability in the governing partial differential equations when introducing a density-dependent flowstress. Geometrically (fixed number of dislocations) and kinematically (fixed plastic capacity) invariant changes to the size of the plastic inclusion are investigated. The formation of a boundary layer with reduced plastic slip is observed for the small inclusion in DDD. It is demonstrated that this feature depends on the spatial distribution of dislocations normal to the slip plane and can be mimicked within CDD by introducing a backstress term that is inversely proportional to the (average) spacing between active slip planes.

[1] A. Arsenlis, D.M. Parks, Modeling the evolution of crystallographic dislocation density in crystal plasticity. J. Mech. Phys. Solids, 50, 1979–2009 (2002)

(J7 oral) **Interface controlled devitrification kinetics in a binary Fe-C glass**

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While the Fe-C binary system is not known to be a good glass former, it can readily be produced in this form as thin films via magnetron sputtering. The devitrification behaviour of this alloy is found to be strongly dependent on carbon content and temperature. At low carbon contents (below 20%C) and low temperatures (< 250°C) a regime can be found where the material crystallizes by forming nearly pure bcc iron which then grows by rejecting carbon into the surrounding glass. Interestingly, the kinetics of crystallization appear to be strongly related to the fraction crystallized, the rate of crystallization slowing drastically with time.

In this contribution experimental results will be presented for in-situ TEM observations of crystallization in binary Fe-C glasses as well as ex-situ 3D-APT measurements of phase composition after partial crystallization. In order to help understand the observed behaviour, atomistic modeling is used to look at the processes that control the rate of interface migration with a particular focus on why the rate of interface migration slows with carbon content of the glass.

(J7 oral) **From atomistic simulations towards a mesoscale representation of the absorption of dislocations in grain boundaries**

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Dislocation-grain boundary (GB) interactions are important for the plastic deformation of nanocrystalline and ultra-fine grained materials. Advanced models for the mechanical behavior of polycrystalline metals therefore need to take GBs explicitly into account. Several approaches to include GBs into mesoscale models (dislocation dynamics, strain gradient plasticity models, ...), were recently suggested. Such GB models need information, like the conditions for dislocation absorption, the change of dislocation stress field after dislocation absorption, or on how much dislocation content can be absorbed. Atomistic simulations are uniquely positioned to provide such information and advance our understanding on dislocation-GB interactions.

Here we present results of carefully controlled studies of dislocations interacting with GBs in model bicrystalline samples. The mechanisms during dislocation-GB interaction are studied in quasi-2D and fully 3D samples. The stress signatures of the absorbed dislocations are analyzed and a novel approach to model the effect of the dislocation absorption on the dislocation stress field is proposed. This approach is then presented in the context of higher scale simulation methods, such as continuum dislocation dynamics (CDD) and discrete dislocation dynamics (DDD). The validity of this approach is also discussed in the framework of the strain gradient plasticity. A primary aim of the current study is to provide a better understanding of the role of absorbed dislocation content on the dislocation-GB interactions, including dislocations nucleation, pile-up and pinning.

(J7 oral) **An updated strategy for the ab initio determination of the grain boundary traction-separation curve: probing the kinetic aspects of the problem**

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[1]Université Paris Diderot, France, [2]Université Paris XIII, France

Computationally, the supercell based grain boundary (GB) uniaxial tensile test by aid of first principles methods represents the atomistic cornerstone in a multiscale modeling analysis of this system. Usually regarded as a standard procedure with more than a decade of application, we argue that the conventional determination of the energy-separation curve holds a fundamental outstanding issue concerning the ease by which the GB may be broken. By critically assessing existing strategies for the energy-separation curve determination, and performing our own density functional theory (DFT) based studies probing the kinetic aspects of the problem, we propose an updated general strategy. Results are provided for selected Al GBs, and the impact of our suggested modification of the existing framework is discussed.

(J8 invited) **Continuous modeling of grain boundary structure in a field theory of dislocations and generalized disclinations**

C Fressengeas[1], X Sun[2], V Taupin[3] and P Cordier[2]

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The duality between the discontinuity of the elastic displacement vector and distortion tensor and the incompatibility of the second-order elastic distortion tensor is used to introduce smooth dislocation and generalized disclination fields in a crystalline body. Beyond Volterra's defects (dislocations and disclinations), generalized disclinations are line defects accommodating discontinuities of the elastic distortion across bounded surfaces. In the atomistic description, the discontinuity of the elastic displacement vector and distortion tensor occurring across grain boundaries and interphases is accommodated by the periodic arrangement of atoms in structural units. In the present work, a crossover between this description and the continuous representation of boundaries using dislocation and generalized disclination fields is carried out by building on the discrete atomic positions generated by molecular dynamics simulations. The example of a symmetric tilt boundary in copper is provided. A comprehensive description of the boundary structure in terms of elastic strain and second-order distortion is then derived from the theory of dislocation and generalized disclination density fields. Such continuous modeling of grain boundaries at inter-atomic scale is attractive, not only for the mechanical description it provides, but also because it paves the way for coarse-grained dynamic modeling of polycrystalline media. The theory provides a dissipative dynamic framework for plasticity and phase transformation through crystal defect motion, on the basis of conservation laws for the elastic displacement and distortion discontinuities. It is capable of addressing elastic interactions between dislocations, grain boundaries and interphases, as well as interphase motion and dislocation/grain boundary-mediated plasticity along arbitrary loading paths.

(J8 oral) **A FFT based-method for continuum dislocation and generalized disclination mechanics**

S Berbenni[1], V Taupin[2], K S Djaka[3], C Fressengeas[3] and L Capolungo[4]

[1]CNRS, LEM3 UMR 7239, Université de Lorraine, France, [2]CNRS, LEM3 UMR 7239, France, [3]University of Lorraine, France, [4]MST-8, Los Alamos National Laboratory, USA

A Fast Fourier Transform (FFT) based-method is developed to solve the equations of the field dislocation and generalized disclination (or g-disclination) mechanics for periodic media with heterogeneous elasticity. After prescribing a Nye's dislocation density tensor and a g-disclination density tensor on the pixel (or voxel) grid, the incompatible and compatible parts of the elastic distortion are obtained, respectively, from the resolution of Poisson-type equations and a Lippmann-Schwinger integral equation with incompatibilities in the Fourier space. The equations are numerically solved through an iterative basic scheme based on intrinsic discrete Fourier transforms with centered and rotated finite difference schemes, respectively. For a single pixel regularization of the dislocation and g-disclination densities within the defect core, the elastic fields due to such defects with elastic heterogeneities are accurately obtained by the present method.

(J8 oral) **Role of lattice curvatures on mechanical response of nanocrystalline materials using a couple stress elasto-viscoplastic fast Fourier transform framework**

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In polycrystalline materials, lattice curvatures manifest themselves at the location of rotation gradients such as grain boundaries (GBs) and triple junctions (TJs). Thus far, continuum based simulation studies performed on bi-crystalline and tri-crystalline structures have highlighted the significance of curvatures in capturing the local geometry, stress state, and non-local dynamics of GBs and TJs. The next step is to develop a suitable framework that allows understanding the role of these curvatures on the mechanical response of polycrystalline aggregates, especially those of nanocrystalline materials where plasticity mechanisms are predominantly GB mediated.

To that end, a couple stress continuum based elasto-viscoplastic fast Fourier transform (CSEVP-FFT) framework is developed and applied to study the role of curvatures on local meso scale and effective macroscale mechanical response of nanocrystalline materials. This framework allows characterizing the initial microstructure with grain boundary curvatures that capture the boundary structure and defect content. Uniaxial loading simulations reveal that local Cauchy stresses are generated from (i) applied macroscopic boundary conditions and (ii) initial curvatures. Furthermore, these Cauchy stresses are accommodated by elastic and plastic curvatures in addition to strains. In some plastically deforming grains, Cauchy stresses generated from initial curvatures result in the activation of slip systems that do not fulfil the Schmid criterion. The combined effect of these meso scale phenomena results in the grain size dependent softening response in nanocrystalline materials known as the inverse Hall-Petch effect. This size dependent response is a natural consequence of the modeling framework and does not involve any ad hoc assumptions.

(J8 oral) **Grain boundaries in Field Dislocation Mechanics: a thermodynamic formulation for the tangeantial continuity condition of distortion at the interface**

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In the material by design paradigm and at a small scale, the treatment of interfaces is an important concern. Indeed, those interfaces often dictate the macroscopic behavior.
To tailor the interfaces to our need, one has to establish precise and predictive models.

In the field dislocation and disclination framework, grain boundaries are represented by an arrangement of dislocations, and/or disclinations dipoles.
Tangential continuity of the distortion tensor derives from the conservation of the Burgers vector over the interface. If the interface is considered vanishingly thin, this is equivalent to an absence of surface dislocations.
However, at small scale, interfaces have finite thickness, and modeled as such in the present work.

A thermodynamic framework is proposed to study the impact of the tangential continuity condition.
In this formalism, the surface dislocations are replaced by the Nye dislocation tensor distributed in a thin region around the grain boundaries.

A surface dislocation energy term is used to limit, or not, the storage of surface dislocations in the interface, which is shown to lead to a back stress term in the driving force for plastic straining.
Simulations of polycrystals are performed by FFT to highlight the resulting non local impact, as well as the long range and size effects.

(J8 oral) **Effects of interfaces and grain-to-grain interactions on shear banding in Al-Cu-Li rolled sheets**

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Crystal plasticity finite element simulations of tensile tests on thin polycrystalline samples with grain orientations representative of the microstructure in Al-Cu-Li rolled sheets are carried out to study the influence of grain-to-grain interactions on plastic strain localization. Anisotropic work-hardening and rate-sensitivity of the material behavior are assumed. The grains are modeled as thin platelets in the through-thickness direction, elongated in the rolling and transverse directions. The only distinctive feature of the present simulations with respect to standard crystal plasticity calculations is the enforcement of tangential continuity conditions on the elastic and plastic distortion rates along grain boundaries, which introduces grain-to-grain interactions and renders the simulations nonlocal. Whereas standard crystal plasticity calculations do not predict any significant plastic strain pattern, slanted shear bands spontaneously emerge throughout the sample in the simulations involving tangential continuity, in agreement with experimental observations. Also in agreement with experimental data, shear banding is delayed when the tensile axis shifts from rolling to transverse direction, and the trend to shear banding is enhanced when grain thickness is decreased, particularly in loading along the rolling direction.

(J9 invited) **Grain boundary plane structure-property relationships and fundamental zones**

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A full crystallographic description of a grain boundary requires 5 parameters, 3 for misorientation and 2 for boundary plane orientation. Typical characterizations focus on misorientation, but boundary plane plays an important role in structure-property relationships. The presented work focuses on describing the GB crystallography, including boundary plane orientation, in fundamental zones and demonstrates that structure-property relationships naturally emerge from this form. Structure-property relationships of energy, excess volume, and mobility are demonstrated for a range of GB types. The fundamental zone representation also suggests possible trends over the full 5D space among similar disorientation axis grain boundaries. Finally, the various mobility trends in $\Sigma 3$ grain boundaries are explained in the context of this fundamental zone representation.

(J9 oral) **Continuous modeling of a grain boundary in MgO and its disclination induced grain-boundary migration mechanism**

X Sun[1], P Cordier[1], V Taupin[2] and C Fressengeas[2]

[1]Université Lille 1, France, [2]Université de Lorraine, France

Grain boundaries (GBs) are thin material layers where the lattice rotates from one orientation to the next one within a few nanometers. Because they treat these layers as infinitely thin interfaces, large-scale polycrystalline representations fail to describe their structure. Conversely, atomistic representations provide a detailed description of the GBs, but their character remains discrete and not prone to coarse-graining procedures. Continuum descriptions based on kinematic and crystal defect fields defined at interatomic scale are appealing because they can provide smooth and thorough descriptions of GBs, recovering in some sense the atomistic description and potentially serving as a basis for coarse-grained polycrystalline representations. In this work, a crossover between atomistic description and continuous representation of a MgO tilt boundary in polycrystals is set-up to model the periodic arrays of structural units by using dislocation and disclination dipole arrays along GBs. The strain, rotation, curvature, disclination and dislocation density fields are determined in the boundary area by using the discrete atomic positions generated by molecular dynamics simulations. Then, this continuous disclination/dislocation model is used as part of the initial conditions in elasto-plastic continuum mechanics simulations to investigate the shear-coupled boundary migration of tilt boundaries. The present study leads to better understanding of the structure and mechanical architecture of grain boundaries.

(J9 oral) **Investigating the Interplay between Grain Boundary Facet Junctions and Interfacial Dislocations**

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Grain boundaries often develop faceted morphologies in systems for which the interfacial free energy depends on the boundary inclination. Although the mesoscale thermodynamic basis for such morphological evolution is well established, less clear are the atomic-scale influences on the behavior. In this presentation, through a combination of atomistic simulations and electron microscopic observations, we examine in detail the structure of an asymmetric Σ=5 [001] grain boundary in body centered cubic (BCC) Fe. The observed boundary forms a hill-and-valley morphology composed of nanoscale {310} and {210} facets. Our analysis clarifies the atomic structure of the {310}/{210} facet junctions and shows how they are related to the elementary structural units of the symmetric {310} and {210} boundaries. Our analysis also identifies the presence of an array of secondary grain boundary dislocations that are localized to the facet junctions. Analysis of the Burgers vectors of these defects, which are of type (1/5)[310] and (1/5)[120], shows that the defect density is consistent with that required to accommodate a small, observed angular deviation from the exact Σ=5 orientation relationship. These observations and analysis suggest an important role for secondary grain boundary dislocations in dictating the grain boundary facet length scale and help to link our microscopic understanding of atomic structure to the macroscopic descriptors of interfacial inclination and misorientation.

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(J9 oral) **Connecting radiation damage evolution and grain boundary structure**

B Uberuaga

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Much of the fundamental research on nuclear materials is focused on improving radiation tolerance, to enable both higher burnup in fission reactors as well as developing materials that can contain the plasma for fusion reactors. One route that has been proposed to improve the radiation resistance of nuclear materials is to go nano. The high density of interfaces in nanomaterials is expected to provide sinks for radiation-induced defects and thus enhance the tolerance of the material. However, despite extensive research over many years, there are still fundamental questions about the interaction between interfaces and radiation-induced defects. Here, using Cu as a model material, we use both molecular dynamics and long-time simulation methods (including accelerated molecular dynamics and object kinetic Monte Carlo) to examine how grain boundaries influence radiation damage evolution. We focus on the role of boundaries in the initial defect production stage during collision cascades and the longer term fate of those defects. We find that grain boundaries do not always promote enhanced tolerance. Further, we show that complex interactions can arise between damaged boundaries and residual defects. Finally, we connect defect mobility in grain boundaries to sink efficiency. We find that in-boundary annihilation of defects, which is ultimately controlled by in-boundary defect mobility and depends on both the nature of the defect as well as the grain boundary character, has an important influence on the sink efficiency of the boundary. We discuss the ramifications of these results on the radiation tolerance of nanomaterials more generally.

(P2.34) **Ab initio study of Cu diffusion along the Sigma 5 (012)[100] grain boundary in TiN**

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Titanium nitride is a material that is often used as a diffusion barrier in microelectronic devices [1]. Its primary role is to prevent copper contacting silicon, which leads to the formation of Cu3Si and thus undermines the device integrity. The TiN film can, in principle, be deposited as a single-crystal or in polycrystalline form. Recently, some progress has been made in understanding the Cu diffusivity in single-crystalline TiN [2,3]. On the other hand, for poly-crystalline TiN films, the situation is less clear. While experimental diffusion data at high temperatures are consistent with theoretical predictions employing a bulk mechanism, the diffusion at lower temperatures is presumably most prominent along the grain boundaries. However, the details of the GB diffusion, such as the precise mechanism, are poorly understood. In this work we present results of an ab initio study of Cu diffusion along a selected GB in TiN, namely Sigma 5(012)[100]. The study includes: 1) Vacancy and Cu segregation to the GB, and their connection to the possible diffusion mechanisms; 2) Migration barriers for a number of diffusion mechanism; 3) Comparison of the calculated GB migration barriers to the available experimental and theoretical data.

[1] M.-A. Nicolet, Diffusion barriers in thin films, Thin Solid Films 52, 415 (1978)
[2] L. Tsetseris et al., Migration of species in a prototype diffusion barrier: Cu, O, and H in TiN, Applied Physics Letters 94, 161903 (2009).
[3] A.S. Bochkarev et al., Ab initio study of Cu impurity diffusion in bulk TiN (in preparation)

(P2.41) **Diffusion bonding of Cu atoms with molecular dynamics simulations**

A Xydou[1], S Parviainen[2], M Aicheler[2], F Djurabekova[2]

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The diffusion bonding method is used for the fabrication of the Accelerating Structures (AS) which are made of copper disks and are one of the main components in the design of future linear collider. In order to address several questions that are related to the bonded joint, the diffusion bonding technique is examined by means of molecular dynamic simulations. A nano-void, corresponding to the initial surface roughness, is inserted between the grains of different and same crystallographic orientations and the bonding conditions, like the pressure and the high temperature are applied. The size of the void varied from 3.5 to 6.5 nm, while the temperature range that is used is 0.7 T_m up to 0.94 T_m.

The voids within a single crystal are thermally stable up to 0.94T_m and the effect of pressure range that is examined is 300 - 800 MPa. The time required for a void to close follows an exponentially decreasing distribution. On the other hand, the voids in a grain boundary (GB) become thermally unstable at temperatures far below the T_m. This instability leads to the void's closure in the examined temperatures before the application of pressure. The closing time presents an exponential dependence on the temperature and the diameter of the void. The diffusion coefficient in the GB was found to be higher than in the surface layer of the void. The activation energy for the GB diffusion which is calculated through the diffusion coefficient of the GB agrees with the value given by Coble.

(P2.42) **Numerical simulations of twin formation and extension in thin metallic film**

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The basic mechanisms of plasticity in face-centred cubic materials are well known in bulk materials. However, several studies have shown that at the nano-scale, some mechanisms can induce surprising mechanical properties when compared to bulk behaviour. Nano-twinned or nano-layered metals for example, are known to have ultra-high mechanical strength, due to the interactions of interfaces or twin boundaries with dislocations [1]. Atomic simulations are particularly adapted for studying the plasticity mechanisms, as mechanical twinning, since they allow their visualization at the atomic scale.

While many atomistic simulations studies have been focused on the interaction between interfaces and dislocations, our study differs in the choice of crystallographic orientations, specifically designed to facilitate twin formation. In that context, we analyse, in a thin face-centred cubic metallic film, the competition between free surfaces and interfaces for twin nucleation under applied stress, as well as the influence of an interface on twin propagation. The chosen orientation also allows the introduction of specific surface defects, which can act as dislocation sources under mechanical stress.

Our study highlights the role of a twin boundary and bimetallic semi-coherent interfaces, on mechanical twinning and particularly on twin extension. We show in particular that the interaction between a newly nucleated twin and a twin boundary causes the formation of a Lomer dislocation. In the case of a bimetallic interface, residual dislocations lead to a local change of the interface [2] which is expected to influence the growth of twin.

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(P2.43) **Investigating alpha and beta phases in Ti-6Al-4V using crystal plasticity finite element modeling**

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There is a growing need to understand the damage mechanisms in two-phase titanium alloys due to their widespread use in the aerospace industry (especially within gas turbine engines), variation in their properties and performance based on their microstructure, and their tendency to undergo premature failure due to dwell and high cycle fatigue well below their yield strength. Two-phase titanium alloys occur in a number of microstructural forms depending on the nature of processing and heat treatment they have undergone. This work focuses on Ti-6Al-4V with a duplex microstructure, consisting of α (HCP) and β (BCC) phases arranged in a lamellar arrangement via a continuum description of dislocation motion. A crystal plasticity finite element (CPFE) model for a polycrystal that incorporates the microstructural features such as α-β colonies is presented in this work. Behaviour of the slip systems at the single crystal level, influenced by dislocations such as dislocation motion and hardening due to pile-up, is taken into account at the continuum scale within the model formulation. Most crystal plasticity models in literature for Ti-6Al-4V homogenize the α and β phases or neglect the β phase due to its low volume fraction. In the CPFE model presented in this research, the α and β phases are modeled explicitly in order to capture the anisotropy between them, which is very important to understand fatigue and damage. The implications of this work look at linking microstructural features to damage in two-phase titanium alloys.

(P2.44) **A combined DFT and tight-binding study of stability and early stage oxidation on Ni-Cr binary alloy with the variation of chromium content**

N Das and T Shoji

Tohoku University, Japan

Nickel-based alloys are important to modern industry because of their ability to withstand severe operating conditions. Oxidation is an inevitable process of materials when the metal is exposed to the environment. In this study, DFT calculations were performed by the VASP code. Simultaneously, semi-empirical code ‘colors’ employed to analyze the interface reaction dynamics in high temperature environments. The cohesive energy (Ecoh) of bulk Ni and Ni (111) surface was 4.57 eV and 4.44 eV, respectively, and the energy value was gradually decreasing with increasing Cr concentration. There is a clear preference for the lower cohesive energy atoms to occupy the surface and leave higher cohesive energy atoms in the bulk. Consequently, the metal surface becomes less protective. Additionally, Cr on top of surface layer showed the positive segregation energy, which reveals antisegregating from the top layer and the energy value was increasing with increasing Cr concentration, suggesting that doping of Cr on sub-surface is energetically unfavourable. QCMD result showed that the highest MSD value of O was attained by the Ni surface and the diffusivity of O is gradually decreasing with increasing of Cr concentration in each layer. Doping of Cr on the first layer was more effective than that of sub-surface layers. For random doping, the surface with 30% of Cr was the most protective from oxidation view point. It reveals that the localized Cr formed a preferential bond with oxygen resulting in the initiation of a passive film formation that can protect the surface from further oxygen diffusion.

(P2.45) **Dislocation nucleation from grain boundary: An accelerated MD study**

J Du[1], Y-J Wang[2], Y-C Lo[1], L Wan[3] and S Ogata[4]

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Dislocation nucleation from grain boundaries (GBs) becomes one of the dominant plastic deformation mechanisms at nano-scale materials. Dislocation nucleation at room-temperature is an infrequent event that is far beyond the time-scale of normal molecular dynamics (MD). Here, a partial dislocation nucleation mechanism transition is uncovered for the GBs with E structural unit in Cu under uniaxial tensile deformation using free-end nudged elastic band method and adaptive-boost accelerated MD. The nucleation event can be accelerated to the time-scale of experiments, such as nucleating one dislocation per second at 300K. With increasing stress, the dislocation nucleation mechanism transits from a shuffling-assisted nucleation to a non-shuffling collective nucleation with time-scale ranging from seconds to picoseconds. The relationship between the mechanism transition and the intrinsic properties of GB, such as the free volume and grain boundary energy, is discussed based on the minimum energy paths of dislocation nucleation of the different coincidence sit lattice GBs. The transition of nucleation mechanism leads to a nonmonotonic decreasing activation volume with increasing stress. At low stress level where dislocations nucleate at a frequency of experimentally relevant time-scale, the activation volume decreases with increasing temperature, which is in agreement with the experimental observations. This study provides comprehensive insights into the complicated competition of dislocation nucleation mechanisms from GBs over a wide range of time-scale.

(P2.46) **Special interfaces in hexagonal metals**

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Institute of Physics AS CR, Czech Republic

In addition to dislocations, several types of interfaces including twin boundaries have essential impact not only on mechanical properties but on general behaviour of hexagonal metals. The interfaces in hexagonal lattice will be analysed and it will be shown that besides the symmetrical interfaces with exceptional properties, there are other non-symmetrical interfaces possessing certain unique structures giving them special properties. The results of atomistic simulations will be presented and compared with the geometrical criteria for the interface classification.

(P2.47) **Temperature-dependent atomistic plasticity in silicon carbide crystal: molecular dynamics model of nanoindentation**

K-I Saitoh[1], K Nishimura[2], T Sato[1], T Hanashiro[1], M Takuma[1] and Y Takahashi[1]

[1]Kansai University, Japan, [2]Natural Institute of Advanced Industrial Science and Technology (AIST), Japan

Use of silicon carbide (SiC) material is now developing in high-power and high-temperature electric devices. However, the process of machining or cutting of SiC crystal is found more troublesome than that in silicon (Si) single crystal. One reason is that mechanical behaviour, in particular "plasticity", of SiC crystal is not essentially (i.e. atomically) known. In this study, to clarify the plastic deformation mechanism of SiC crystal, molecular dynamics (MD) simulations of a nanoindentation model of cubic SiC crystal using a nano-sized spherical indenter is performed. We are using a Tersoff-type interatomic potential function after we checked and selected out of some parameter sets suitable for Si-related systems. Transition from elastic deformation to plastic deformation is clearly confirmed by so-called "pop-in" event in the load-displacement curves of nanoindentation. We are able to identify crystalline slips and defects in SiC by a novel type of structural analysis method using sub-lattice of Si or C which is based on common neighbour analysis. In the plastic process of SiC, first, dislocations on {111} slip planes appear, and then defects are detected in characteristic shape of square pyramid when the pop-in behaviour occurs. Increase of indenter depth causes initiation and development of dislocation loops along {111} planes. Temperature dependence of plastic behaviour is as follows. The same level of resolved shear stress causes a nucleation of dislocation. In lower temperature, dislocation loops move exclusively to lateral directions parallel to the surface, while in higher temperature they spread even more into the depth of SiC.

(P2.48) **Evaluation of stress concentrations induced by dislocation microstructures onto grain boundaries in Al polycristal by dislocation dynamics**

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In polycrystalline materials, fracture is often initiated at weak spots of the microstructure, such as Grain Boundaries (GBs), triple junctions or around precipitates. Crack initiation at GBs is affected by several parameters such as temperature, plastic activity within grains, dislocation accumulations at GBs, or the presence of impurities. Among these impurities, hydrogen atoms diffuse toward GBs and reduce their cohesive energy (phenomenon known as Hydrogen Embrittlement). In consequence, the exact conditions, e.g. when and where debonding will start within a given microstructure, are still not precisely known. This phenomenon is furthermore strongly dependent on the local stress field, which cannot be evaluated using J2 or crystal plasticity-based finite element method (FEM) computations.

This work aims at improving our understanding of the hydrogen-assisted intergranular fracture through the mapping of stress concentrations at GBs in Al multicristals, induced by deformation microstructures. To this goal, Dislocation Dynamics (DD) simulations coupled with FEM are employed to reproduce in 3D the dislocation accumulation observed at GBs. The influence of slip conditions, GB geometry and cross-slip activity is evaluated. These results are discussed in conjunction with atomistic data on the resistance of GB to local stress state.

(P2.49) **Atomic-scale modelling of the Ni-S system via a comparative study of semi-empirical interatomic potentials**

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The Nickel – Sulfur system is a well – known example of segregation of non – metal impurity (S) at the grain boundary (GB) of a metallic system (Ni), inducing the embrittlement of the latter [1]. In the last decade, atomic – scale modeling has suggested two complementary scenarii, that partly unveil the reasons for such embrittlement: (i) first – principles techniques suggest a strong alloy effect due to the repulsion between the first few S impurities introduced [2] and (ii) reactive force fields Molecular Dynamics simulations underline the possibility of an amorphous interface [3]. But both approaches stand for either an isolated small (80 atoms) GBs or a very large polycrystalline material.

To understand the possible coupling between alloy and elastic effects it is necessary to clarify the role of GB anisotropy on adsorption anisotropy. We propose a tight – binding formalism to be compared to current interatomic potentials available for pure Ni and Ni-S systems, in particular regarding thermodynamical and elastic bulk properties.

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(P2.50) **Multiscale modeling of interfaces and their effect on the mechanical and thermodynamic properties of crystalline materials**

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Solute-grain boundary (GB) interactions play a critical role in the microstructure development of many materials. Density functional theory (DFT) is a very desirable tool for studying these interactions because of its high accuracy and the ease with which different solute species may be investigated. Unfortunately, the high computational cost of DFT calculations limits us to a very small set of high-symmetry boundaries. Quantum mechanical/molecular mechanical (QM/MM) multiscale methods provide a tool for bypassing this problem: full chemical interactions can be captured in a small quantum domain of interest (e.g. in the neighbourhood of a solute atom) while long range elastic interactions are treated by a classical atomistic representation. Such methods are ideal for studying the behaviour of solutes in low-concentration at GBs.

We have developed an improved QM/MM method which is amenable to the complex situation when a structural defect passes through the quantum-classical coupling domain, as is the case in GB calculations. This improved method is first benchmarked against pure-DFT using Pb- and Mg-binding to a $\Sigma 5$ boundary in Al. Next, we calculate the binding of these solutes to a selection of sites at a general, low-symmetry Al tilt boundary using only QM/MM; such a boundary is completely beyond the reach of traditional DFT. These QM/MM results are then used to evaluate the performance of two classical atomistic potentials and also to test the extensibility of a simplified model for GB-binding that was found to work well at a high-symmetry boundary in Mg.

Symposium K

(K1 invited) **Ordering and surface segregation in miscible Nanoalloys: cases of Co-Pt, Pd-Au and Pd-Pt**

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Ordered structures in alloys induce physical properties as the increase by a factor of ten of the magnetocrystalline anisotropy between the pure metal and the ordered alloy. This property has been intensively exploited in nanoalloys for high density data storage. However we know that ordering in nanophases can be disturbed by surface segregation leading to chemical frustrations.

Ordering and surface segregation are fundamental aspects of the chemical structures in miscible nanoalloys. A lot of studies have been performed on nanoalloys with immiscible elements (Cu-Ag [1], Ni-Ag, Co-Ag) leading to rationalized analyses as core-shell or Janus-like structures [2], but there is much less similar studies concerning miscible systems. On the basis of three different systems with decreasing ordering tendency we show very different behaviours starting with a strong ordering tendency (Co-Pt [3]) where surface segregation effects are weak, to moderate ordering tendency (Pd-Au [4]) where surface segregation leads to almost perfect core-shell structures, and to finish by a weak ordering tendency (Pd-Pt [5]) which consists of a solid solution where the slight surface segregation leads to multiple-shell structures near the surface.

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(K1 oral) **Experimental and modeling comparison in atom segregation of Ag-based bimetallic clusters**

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We can distinguish three main driving forces in order to predict the nature and the quantity of the segregating species in a binary alloy: the differences in surface energies and radii of the two elements (mismatch-effect), and their ability to mix in the bulk. In Ag-Co system, we can predict a surface segregation of silver since Ag presents lower surface energy and larger size (to minimize elastic-energy), in addition to the very large miscibility gap in wide ranges of temperature and concentration, without alloyed phases.

To the nanometer scale, the size reduction favors a segregation behavior by surface and core contraction effects that can be opposed to kinetic trapping effects induced by the growth mode. In our works, mobility and stability of Ag-based supported nanoalloys (Ag-Co and Ag-Pt) were studied through modeling and experimental in situ investigations of structural arrangements and especially, the stability of core-shell, janus or alloyed configurations.

Experimentally, morphological and structural evolutions of clusters are followed by HRTEM/EFTEM/HAADF techniques combined with in situ and real time wide- and small-angle X-ray scattering: the metastable deposition mode at room temperature, i.e. by depositing Co above an Ag core, and the more stable reverse deposition mode until their equilibrium state obtained by thermal activation. The equilibrium and non-equilibrium structures were simulated using Monte Carlo methods in a semi-empirical tight-binding approach in the second-moment approximation for various compositions and sizes. Especially, the nanosize effect on the stability of icosahedral structure was studied in comparison to the crystalline truncated octahedral structure.

(K1 oral) **Multi-scale modeling of core-shell Fe@Au nanoparticles**

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Magnetic metallic nanoparticles (NPs) provide promising applications, especially in biomedicine. The NPs properties can be tuned by controlling the NPs size, shape and composition. For biomedical applications, the problem of the NP oxidation can be overcome by passivating the surface with a bio-compatible metal such as gold. Experimentalists from CEMES (Toulouse) have managed to grow highly facetted Fe@Au core-shell NPs of ~8-10 nm using vapor phase deposition techniques. These NPs display an original polyhedral core–shell morphology in which a Fe nanocube core acts as a nanosubstrate for the epitaxial growth of gold islands with a truncated pyramid shape. Interestingly, pure Fe NPs grown in the same conditions mostly exhibit a rounded shape, and the cubic morphology only appears after Au coverage. In this work, we present a multi-scale computational modeling of these objects with the aim of understanding the key parameters that control their morphology and their properties. Structural and electronic properties of the interface between the core and the shell and of the NP surface have been investigated by DFT as a function of the shell thickness. From these results, we built a Fe-Au interaction potential of the EAM type, which was used to study the evolution of the NP morphology as a function of size and Fe/Au volume ratio. Finally, finite element modelling in the framework of the linear elasticity has been carried out to investigate the relative stability of the symmetric and asymmetric NP shapes as a function of size.

(K1 oral) **A Cahn-Hilliard approach to modelling phase separation in bimetallic nanoparticles**

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[1]University of Birmingham, UK, [2]Institute of Electronics, Bulgarian Academy of Sciences, Bulgaria

Bimetallic nanoparticle systems exhibit rich self-assembly behaviour, and an understanding of the factors affecting their structure is crucial for developing applications. One example is the Cu-Ag system, which has been shown to undergo a transition from core-shell to side-segregated quasi-Janus particle structure as the particle size increases.

Atomistic computational methods are restricted in terms of the number of atoms being taken into account, and although they are able to predict the core-shell to quasi-Janus particle transition, they are not capable of modelling the transition to bulk behaviour, using current supercomputers. In order to overcome this limitation, we present a continuum-scale approach, based on the ternary Cahn-Hilliard equations, to modelling phase separation processes in bimetallic nanoparticles. The third component in the ternary system is taken to be vacuum, such that we are able to simulate bimetallic nanoparticles without any need to impose restrictions on the nanoparticle boundary. Strain effects, due to lattice mismatch, are introduced via a coupling with the Navier-Lamé equations of elasticity. A semi-implicit Fourier spectral scheme is used to solve the Cahn-Hilliard system, and the Navier-Lamé equations are solved, at each time step, using an iterative method in Fourier space. The use of this diffuse-interface approach allows the simulation of significantly larger systems than currently feasible with atomistic methods. The method is able to capture the various effects observed previously in experimental work and in atomistic simulations.

(K1 oral) **Modeling finite-size effects on phase-separation transitions in nanoalloys**

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Ben-Gurion University of the Negev, Israel

Phase-separation second-order transitions in binary nanoalloys (NA) consisting of up to ~70,000 atoms, are modeled focusing on the unexplored issue of finite-size scaling in such systems, including inner interface and shape effects. Our approach is based on mean-field analytical expression for the Ising model free energy [1,2] that facilitates highly efficient computations furnishing comprehensive data for fcc rectangular NAs. These are summed up in intra- and inter-particle scaling plots as well as in nanoalloy phase separation diagrams. Plots of shifts in the critical temperature of transition from Janus-type intra configurations to solid solution vs. correlation-length related interfacial thickness and vs. NA size reflect power-law behavior with the same critical exponent, ν=0.83. A refined analysis reveals size-dependence of ν attributed to interfacial effects that are absent in the inter-particle transitions. In both cases, extrapolation that bridges the gap to very large particles yields ν=1 associated with free surface effects (as compared to 0.50 obtained under bulk-like periodic boundary conditions). Beyond these distinct findings that are consistent with other finite-size-scaling predictions, e.g., for magnetic particles and films, this study indicates the key role of surface-area to volume ratio as effective-linear-size, revealing a universal, particle-shape independent, nano-scaling of the critical temperature shifts.

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(K2 invited) **Experimental atomic arrangements in size-selected clusters - a benchmark for nanoscale modelling**

R E Palmer

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In his 1959 lecture "There's plenty of room at the bottom" Richard Feynman expressed a vision of making materials by arranging the atoms. Atomic clusters were in his thoughts. In this talk I will (i) explore how far we have come in realising the route to new functional materials via deposition of size-selected atomic clusters with 3D structural control, while at the same time (ii) laying down an experimental benchmark for theoretical modelling of nanoscale systems.

On the fundamental side one current frontier is the question of the *metastability* of the clusters themselves. New techniques like aberration-corrected scanning transmission electron microscopy (ac-STEM) are only now being applied to soft-landed, size-selected clusters. Dynamical manipulation experiments [1,2], which probe the transformation of metastable isomers into more stable configurations, and reaction-exposure experiments, which probe the response of the nanocluster structures to catalytic conditions, will be treated. Such experiments provide a body of data to stimulate and constrain computational models and are readily extendable to binary systems.

The talk will conclude with a brief discussion of new efforts to scale-up dramatically the rate of cluster generation, which promise significant future impact in practical technologies, such as catalysis, metrology and biomedicine.

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(K2 oral) **Ageing of nanoalloys: Formation and dissolution of the onion-like nanostructure**

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For an alloy, it is often possible to observe different configurations depending on the experimental process. The non-equilibrium configurations should evolve towards the thermodynamically stable configuration for sufficient long time. When the physical properties of nanostructures are interesting the question of their life-time is of great interest.

In this study we explore the time evolution of non-equilibrium bimetallic nanoparticles toward equilibrium configurations using both Kinetics Monte Carlo (KMC) simulations and a kinetic mean-field description which provides the time evolution of the concentration for *each site* called MFA-SK approach (Mean-Field Approximation, Site Kinetics), based on the same atomic model. We consider a cuboctahedron nanoparticle of 309 atoms ($Cubo_5$). Energetic parameters of the rigid lattice pair interaction energy model are fitted to represent the Cu-Ag system characterized by a strong tendency to phase separate and the tendency of Ag atoms to segregate at the surface.

Starting from an initial configuration with a random distribution of the two species, the kinetics exhibits two different evolution pathways at low temperature. Either the nanoparticle evolves directly towards its equilibrium core-shell structure or the nanoparticle passes through a metastable onion-like configuration on its way. Using the MFA-SK approach, we analyze in detail the formation and the dissolution of the onion-like structure. We show that the formation of the onion-like structure occurs when the initial core concentration is slightly enriched in Ag, and we identify the main diffusion paths during the dissolution.

To conclude we compare the present behavior to the one observed for thin films.

(K2 oral) **investigating structural transitions in metallic nanoalloys via Metadynamics**

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Investigating the (meta)stability of nanoarchitectures is paramount to nurture their application in a broad range of fields, from catalysis to biomedicine. Indeed, the peculiar and captivating chemophysical properties of metallic and bimetallic nanoparticles depend on their size, shape and chemical ordering [1]. Generally, structural transitions in metallic nanoclusters are rare events, thus enhanced sampling techniques are needed to access the characteristic timescales of these processes. Recently, we demonstrated how the Metadynamics[2] algorithm, with specifically tailored collective variables based upon the cluster pair distance distribution function, can be used to effectively reproduce solid-solid transitions in mono and bimetallic nanoparticles [3]. After presenting our methodology, transition pathways and free energy barriers for numerous structural transformations, in a variety of systems, are discussed. The universality of solid-solid transitions via Lipscomb's Diamond-Square-Diamond mechanisms [4] in "magic size" monometallic clusters is addressed for a variety of sizes and across the periodic table. For the first time, we evidence the existence of three transition pathways connecting decahedra towards crystalline motifs. Mismatch and chemical ordering constraints which hinder the above listed rearrangement mechanisms in bimetallic nanoalloys are examined, further considering the role of atomic intershell and surface diffusion during chemical reordering [5]. Finally, preliminary result on supported metallic nanoparticles are discussed in the light of a new family of "layer-by-layer" structural transitions.

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(K2 oral) **New designed synthesis of metallic nanoparticles and nanoalloys**

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Different chemical processes, either at high or at low temperature, have been used to synthesize cobalt nanocrystals and platinum derivate nanoalloys Co_xPt_{1-x} and Pd_xPt_{1-x}. Design of new-molecular precursor allows control the nanocristallinity of metallic nanoparticles, as an example pure HCP cobalt nanocrystals ferromagnetic at room temperature can be easily synthesized for the first time. It also demonstrate the nanoscale effect on the formation of Pd_xPt_{1-x}. Furthermore it is evidenced that the chemical route can control the nanocrystallinity of Co_xPt_{1-x}. The order/disorder phase transition induced by annealing has been investigated depending on the route of synthesis. It is demonstrated that the high temperature chemical synthesis allows stabilization of the fcc structure of the native nanoalloys while the soft chemical approach yields mainly poly or non crystalline structure. As a result the approach of the order/disorder phase transition is strongly modified as observed by high-resolution transmission electron microscopy (HR-TEM) studies performed during in-situ annealing of the different nanoalloys. The control of the nanocrystallinity leads to significant decrease in the chemical ordering temperature as the ordered structure is observed at temperatures as low as 420 °C. This in turn preserves the individual nanocrystals and prevents their coalescence usually observed during the annealing necessary for the transition to an ordered phase.

(K3 invited) **Computational design of nanoalloys using DFT calculations, genetic algorithms and machine learning**

T Vegge[1], P C Jennings[1], S Lysgaard[1], H A Hansen[1] and T Bligaard[2]

[1]Technical University of Denmark, Denmark, [2]SLAC National Accelerator Laboratory, USA

Nanoalloys have been found to display highly promising catalytic properties for a range of chemical and electrochemical reactions, e.g. Pt-based nanoalloys for the oxygen reduction reaction (ORR) in fuel cells and Cu-based nanoalloys for electro-reduction of CO_2 (CO2RR) into fuels and chemicals. The activity, selectivity and stability of the catalysts depends specifically on the composition, structure and ordering of the nanoalloys, and the ability to predict and optimize these properties *in silico* holds great potential.

Here, we combine interatomic potentials and density functional theory (DFT) level calculations with genetic algorithms (GA) and machine learning (ML) to accelerate the search for the compositions, which provide the most stable and catalytically active nanoalloys. Traditionally, a GA would allow the search to be performed for optimisation of a single variable, e.g. stability or activity, but the presented MLGA approach allows for a multi-objective optimisation to be performed, where two or more variables can be searched simultaneously. The MLGA yields a substantial reduction in the number of minimizations that need to be performed to find a range of structures of interest.

We will present a number of examples for bi- and tri-metallic nanoalloys and core-shell particles, e.g. displaying improved catalytic activity over pure platinum for ORR, and the identification of novel mixed core – mixed shell particles for CO2RR. Finally, we demonstrate that predictive accuracy can be obtained with a computationally fast LCAO mode for the essential molecular chemisorption energies on the nanoparticles.

(K3 oral) **Modeling of complex metal alloys and nanoparticles via multiscale first-principles methods**

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This work is related to DFT based modelling of phase diagrams of complex metal alloys. Most experimental techniques measure average or macroscopic properties of a material and provide only indirect information regarding the atomistic structure so non-parametric ab initio calculations have been used to supplement the missing points in experimental databases and to guide experimental work to the most interesting areas. In particular, the DFT can provide insight to microscopic features that are manifested as macroscopic properties of a material but the DFT calculations are very time consuming. We have developed a Cluster Expansion (CE) model with heuristic effective cluster interaction selection and Monte Carlo simulations have been used to determine finite temperature configurational phase diagrams for several alloys [1,2]. The modelling of such finite temperature properties provides substantially more information and knowledge than traditional CE studies, which are typically restricted to searching possible ordered ground-state structures at 0 K.

We have recently applied the same method to nanosize clusters. The presentation is mostly of the bulk systems but the resent cluster results will be also addressed.

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[2] J. Teeriniemi, P. Taskinen and K. Laasonen, Modeling of complex ternary structures: Cu–Ni–Pd alloys via first-principles, J. Mater. Sci. 115, 2016, 202–207

(K3 oral) **Structural optimization of Au-Co nanoalloys**

R Ferrando, J-P Palomares-Baez and E Panizon

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Recent experimental results have shown the formation of both phase-separated core.shell Co@Au nanoalloys and of chemically intermixed nanoalloys. The formation of intermixed nanoalloys has fostered some speculation about an increase of equilibrium miscibility at the nanoscale, because the Au-Co system presents a very weak miscibility in bulk crystals. This is still an open issue, which can be clarified by the use of computer simulations.

Here, by using a combination of DFT and atomistic calculations, we demonstrate that intermixed configurations are metastable, the most stable configurations being either core-shell or quasi-Janus. These phase-seperated structures persist well above room temperature, without indication of appreciable increases of miscibility up to the melting temperature.

In the Au-rich regime, we show that a quite small number of Co impurities in Au nanoparticles can cause the structural transition from decahedral/fcc structures to icosahedra with reconstructed surface and then to perfect Mackay icosahedra. This behaviour is attribute to the stress relief caused by small impurities placed at the center of the icosahedral structure.

(K3 oral) **Modelling nanoalloy catalysts: From free to Oxide-supported particles**

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Nanoparticles are ideal for heterogeneous catalysis due to their optimal surface to volume ratio. Alloying two metals can furthermore improve catalytic performance by increasing selectivity, activity or resistance to poisoning due to electronic or geometric effects. Tuning nanoalloy morphology may even enhance catalytic properties by controlling reactivity and/or selectivity. The properties of nanoparticles are also under the influence of a substrate in real world applications. Hence, an accurate description of nanocluster-support interaction is important in nanoalloy catalysis applications and can be achieved by atomistic modelling based on first principle electronic structure calculations.

After a brief overview of our recent work combining Density Functional Theory (DFT) calculations with a genetic algorithm search algorithm to identify the structures and chemical ordering of metal clusters and mixed metal nanoalloys on oxide surfaces [1-3], I will discuss recent studies of fcc-Au-Rh nanoalloys supported on TiO_2(110). Au and Rh are immiscible in the bulk, with alloying only possible at the nanoscale. In experimental studies, TiO_2 has been used as a substrate because it has well defined single phase nanorods (which are suitable for structural analysis) and it is a reducible oxide (which can act as an oxygen reservoir and enhance the catalytic activity) [4]. I will discuss the effect of the substrate on the relative stabilities of different chemical ordering arrangements of the Au-Rh nanoalloys, for a range of compositions. The effect of chemical ordering and the substrate on the strength of adsorption of small adsorbates such as H_2, O_2 and CO.

(K4 invited) **Tight-binding strategy to model the energetics of magnetic alloys and nanoalloys**

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Atomistic simulations are widely used to characterize alloys and nanoalloys of transition metals and a good description of nanoparticle size effects on phenomena like ordering or shape changes has been achieved within energy models like the tight-binding second moment approximation (TB-SMA)[1]. Nevertheless, these types of simulations are still requiring improvements in particular by taking into account the magnetism in energy models, for a better description of segregation and ordering phenomena when interested in magnetic materials [2,3,4]. Tight-binding studies of transition metal based systems deviating from perfect bulk (surfaces, nanoparticles, alloys) are usually based on local charge neutrality rules per site, per valence orbital and per element. Unfortunately, such rules do not hold per spin. Based on a recent work on the environment dependence of magnetic moment and atomic level shifts within the tight-binding approximation [5], we present a methodology to generalize the tight-binding expression of the energy to account for magnetism. This is illustrated in the particular case of CoPt and FeNi alloys, going from pure bulk to alloys and then to alloy surfaces and nanoalloys.

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[3] C. Goyhenex, L. Zosiak, R. Kozubski, G. Tréglia, J. Phys. Cond. Matter, 27 (2015) 455503
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[5] C. Goyhenex, G. Tréglia, B. Legrand, Surf. Sci., 2016, in press

(K4 oral) **Molecular dynamics simulations of self-propagating reactions in Ni-Al multilayer nanofoils**

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Nanometric metallic multilayers (N2M) are made of thin layers (4-100 nm) of metals deposited alternately. N2Ms are structured as a succession of interfaces separated by a few nanometers. The many areas of contact should promote mixing between pure metals and alloying processes. In most cases, it is observed that the ignition temperature of the reaction coincides with the melting temperature of one of the two metals. The mixing is then associated with the dissolution of the solid phase into the liquid one. The Ni-Al reactive foil is chosen as the representative material. By igniting locally one edge of the sample, a self-sustaining reactive front propagates along the foil, without any further supply of heat. The exothermic processes may the interdiffusion of the two metals or the formation of new phases such as intermetallics.

We studied the self-propagating high-temperature reaction that occurs in N2M by means of molecular dynamics (MD) simulations, using an embedded-atom method type potential. MD is a valuable tool to study those systems, since the typical length scale (a few nanometers) corresponds precisely to the scale accessible in the simulation. Beyond the simulation of a large length scale thermal process by MD, this work demonstrates the relation between the dynamics of front propagation and the underlying microscopic processes. Some specific properties such as nucleation and growth of the new intermetallic phase are revealed, while well-established experimental characteristics of front velocity are observed.

(K4 oral) **Nanoalloys as catalysts for fuel cell application: Multiscale simulation and experimental study**

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With respect to the catalysts in fuel cells, Pt-based nanoalloys have been employed to prevent the CO poisoning and to improve the oxygen reduction reaction (ORR) catalytic activity of pure Pt electrocatalysts [1,2]. In addition, Pd-based nanoalloys show higher formic acid oxidation (FAO) activity than commercial Pd/C [2]. Here, first principles density functional theory (DFT) calculations [3-6] and experiments [7-10] have been used to study the oxygen reduction reaction (ORR) and formic acid oxidation (FAO) activity of transition metal nanoalloys.

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(K4 oral) **Metallic nanoclusters on graphene/Ir(111): insights from ab-initio calculations and experiments**

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Fabrication of ordered arrays of metallic nanoclusters (NCs) for catalysis applications is the goal of many efforts. The Moire' pattern of graphene/Ir(111) works as an efficient template to this purpose, in particular for the growth of Pt and Ir based NCs, as predicted by ab-initio calculations and observed for different metal loadings. The chemical and morphological behavior of metallic NCs upon interaction with small molecules of environmental importance such as carbon mono- and dioxide is investigated with atomic- level detail from ultra-high vacuum to near ambient pressure by both spectroscopy and microscopy approaches.

Extensive ab initio calculations give insights into the different nucleation behaviour of Pt and Ir with respect to other metals, such as for instance Cu, and predict that even materials that do not form cluster superlattices can be grown promoting their nucleation through a seeding mechanism with another properly chosen metal.

Support from the Italian Ministry of Foreign Affairs and International Cooperation (MAECI), MIUR, and the University of Trieste (Finanziamento di Ateneo per progetti di ricerca scientifica - FRA2015) is acknowledged.

(K4 oral) **Instability of (100) facets in monolayer-thick core@shell nanoalloys: the emergence of pyritohedral and chiral symmetries**

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Nanoalloys made of weakly miscible elements often present core@shell structures. In these nanoalloys the element which has higher surface energy occupies the interior region and it's coated by the other element (which usually has a smaller atomic size). It has been shown both in simulations and in experiments that the position of the core and the thickness of the shell can vary significantly depending on the mismatch of the lattice parameters and the geometry of the cluster. In many cases the position of the core is found to be preferentially off-centered with a very thin, often mono-layer thick, coating shell. The structure of these shells depend on the local strain, and in turn can influence the catalytic or optical properties of the whole nanoalloys.

Here we present results on a particular class of surface reconstructions: the deformation of (100) surface facets for monolayer-thick core@shell nanoalloys [1]. Due to the presence of large size-mismatch, the (100) surface facets transform into (111) facets. Moreover in high symmetry structures this reconstruction is simultaneous to all facets and present global characteristics; In particular perfect Marks-decahedra rearrange in chiral decahedra, and for Truncated Octahedra (TO) there is a transition from the octahedral (Oh) to the pyritohedral (Th) symmetry. The enhanced stability of these new structures in respect to the non-reconstructed clusters is confirmed at two different level of approximation for the interatomic interactions, i.e. both using semi-empirical many-body potentials and Density Functional Theory.

[1] Emanuele Panizon and Riccardo Ferrando, *to be submitted*

(P1.55) **Silicon nanoparticles grown by magnetron sputtering: crystallisation through hybridisation**

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One of the key challenges in NP technologies is to control simultaneously the size and crystallinity of NPs with as high accuracy as possible, since these two parameters can have a beneficial or detrimental impact on uses for specific applications. For example, crystallisation of Si NPs is of particular interest for the Si-base photovoltaic industry, since it can affect the efficiency of solar cells. Nevertheless, conventional thin-film synthesis systems suffer from inadequate concurrent control of both particle size and crystallinity, especially in the smaller diameter regime. The recently optimised magnetron-sputtering inert gas condensation technique, however, has managed to overcome these limitations. Herein, we will present a brief overview of this method, and show how it allows for a highly desirable flexible design and synthesis of Si NPs of controlled size and structure. The use of alloy targets, or additional sputterring sources, either within the main reactor or beyond it, allow for the design of multi-component hybrid Ag-Si NPs with extra degrees of freedom, those of composition and structure. Clever usage of such tools also enables control over the crystalline structure of the NPs.

(P1.56) **Metal-oxide interface effect on the structure of silver nanoparticles deposited on amorphous silica support**

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In the field of supported nanoparticles, experimental data show that the substrate (*e.g.* amorphous silica) used to support the nanoparticles, despite weakly interacting, may have a non-negligible effect on their properties. A fundamental understanding of these interactions should help to rationalize these experimental data. In particular, this work focuses on the study of the relative stability of the various structures (icosahedron, decahedron and Wulf fcc octahedron) of a silver nanoparticle deposited on amorphous silica.

We use molecular dynamics and Monte Carlo simulations which are expected to be well suited to describe deposited nanoparticles (from few atoms to several thousands) due to the large importance of an atomistic description. These methods rely on effective potentials. The Ag-Ag interaction is modeled by a tight-binding semi empirical potential within the second moment approximation (TB-SMA). The interactions between atoms constituting silica are described by the mTTAM potential. The Ag-silica interaction is treated either within a smooth-wall approximation acting solely on the first atomic layer, or using a site-site Lennard-Jones interatomic potential. The parameters are adjusted on experimental studies and Density Functional Theory calculations performed on simple configurations.

We evaluate the structural stability of the supported silver nanoparticles at zero temperature by energy minimizations, considering icosahedral, decahedral, and Wulf fcc octahedral nanoparticles of various sizes, aspect-ratio and orientations. The effects of surface roughness and temperature are explored, showing that smooth surfaces favor fcc structures, while rough surfaces stabilize decahedral structures. These results are compared with experimental data obtained by vapor deposition on oxidized silicon wafers.

(P1.57) **Ordering and surface segregation in CoPt nanoparticles: from surface alloys to nanoalloys**

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The study of chemical ordering and surface segregation effects in nanoalloys is crucial in the characterization of their properties and applications. Co-Pt are interesting due to the link between atom arrangement and magnetic behavior, for instance in the field of magnetic storage. These systems have the particularity to form ordered compounds in bulk alloy but the question arises if the ordering remains in nano-sized particles and how surface segregation accommodates core ordering. We propose here a theoretical study of surface segregation and chemical ordering.

Extending the previous study on rigid lattice[1], we performed systematic Monte Carlo simulations in semi-grand canonical ensemble on the whole composition range of the Co-Pt nanoalloys with semi-empirical many-body potential within the Second Moment Approximation of the density of states which allows atomic relaxations. This potential has been fitted to ab initio calculations within the density functional theory. We characterized the segregation isotherms for Co-Pt nanoalloys on the whole range of compositions and for different temperatures in order to draw nanoalloys phase diagram. It implies to study the influence of the size and morphology of the clusters. The chemical structure is compared in their core with the bulk phase diagram and in their facets with the (111), (100) infinite surfaces segregation isotherms.

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(P1.58) **Atomic structure and local electronic properties of IrPd nanoalloys**

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The present contribution reports on computational modelling of Ir-Pd nanoalloys. This bimetallic system, which presents a large miscibility gap in the bulk phase, has been little studied in the past. From the experimental viewpoint, IrPd bimetallic catalytic particles appear much more efficient than their Ir and Pd counterparts in the preferential oxidation of CO in presence of hydrogen (PROX) [1]. This synergistic effect has been correlated to Ir - induced inhibition of hydrogen absorption in Pd through nanoalloying. In the aim to provide some insight into the comprehension of this change of catalytic efficiency between pure and alloy systems, we have performed calculations of both the atomic structure, focusing on segregation phenomena, and the local electronic structure.

More specifically, using semi-empirical modelling, namely Tight-Binding at different levels of accuracy, the chemical, crystallographic and electronic structures of bimetallic IrPd nanoparticles are characterized. Atomistic simulations show that core-shell nanoparticles are highly stable, with a strong surface segregation of Pd, at least for one atomic shell thickness [2]. Within self-consistent Tight-Binding calculations founded on the density functional theory, an accurate insight is given into the electronic structure of these materials which have a high potential as catalysts.

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Symposium L

(L1 invited) **Modelling and validation of rapidly solidified alloy structures**

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Rapid solidification of alloys can result in microstructures with extended solubility and reduced microsegregation. Although many models of microstructural evolution have been proposed in the literature, few have been validated using experimental data. This work presents a combined experimental and modelling approach to describe the solidification path of rapidly solidified alloys. In this approach, an experimental eutectic fraction obtained by neutron diffraction is found to be systematically lower than the Gulliver-Scheil predictions for various alloys. Using these experimental values, the eutectic undercoolings are estimated by extending the solidus and liquidus lines of the primary phase into the metastable domain. The eutectic nucleation temperature is determined as the temperature at which the calculated eutectic fraction is equal to the experimental value. These eutectic undercoolings are then incorporated in a coarsening model to estimate the corresponding primary undercoolings. The combined primary and eutectic undercoolings for each droplet are validated by an equiaxed solidification model based on mass and heat balances. The model takes into account diffusion in liquid and solid, as well as the effect of the recalescences occurring after the nucleation of the primary phase and the eutectic structure. A good agreement is found between the output results of eutectic fractions and the corresponding experimental values. The nucleation undercoolings of the primary and eutectic structures are shown to be key parameters in an analysis of the nucleation phenomena.

(L1 oral) **Combining numerical modeling and ultra-fast in-situ TEM for quantitative studies of rapid solidification microstructure evolution dynamics**

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In-situ transmission electron microscopy (TEM) of irreversible reactions can provide important mechanistic understanding and measurements to support computer model development and validation. Exploiting the unique nano-scale spatiotemporal resolution attainable with the dynamic transmission microscope (DTEM) and using Al-Cu as a model system, the transformation dynamics and the microstructure evolution during laser stimulated rapid solidification (RS) have been studied. In-situ TEM revealed crystal growth mode changes under composition-dependent characteristic conditions and facilitated quantitative measurements of locally resolved instantaneous and average transformation interface velocities during the transformations. However, temperature evolution measurements are inherently difficult while performing in-situ DTEM RS experiments. Complementary enthalpy-based numerical modeling has been performed in a multi-physics environment to determine the thermal field evolution during RS. Calculation results have been benchmarked simultaneously against several transformation-related quantitative metrics provided by in-situ TEM experiments. Together with post-mortem micro-analysis, the combined in-situ TEM experiments and numerical modeling of the laser induced transformation processes enabled determination of temperature and microstructure evolution maps. The direct observation-based inputs offer insight to non-equilibrium processes responsible for microstructure development in materials during transformations under far-from-equilibrium, driven conditions typical of laser-assisted rapid solidification processing. Work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory (LLNL) under Contract DE-AC52-07NA27344. Work at LLNL supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Division of Materials Science and Engineering under FWP SCW0974. Work at the University of Pittsburgh supported by the National Science Foundation, Grant No. DMR 1105757.

(L1 oral) **Solidification cracking during Selective Laser Melting of Inconel 738LC: origins and remedy**

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One of the main problems holding back the usage of high-strength, γ'-hardening Nickel-base superalloys in Additive Manufacturing is the formation of microcracks during solidification (hot tearing). To investigate the origins of these defects, we studied specimens made of Inconel 738LC by Selective Laser Melting (SLM), an Additive Manufacturing technique. We prepared Atom-Probe Tomography (APT) specimens from grain boundaries ahead of microcracks and study the composition profiles across high-angle grain boundaries and low-angle grain boundaries. Even though the high cooling rates encountered in SLM are often said to induce rapid solidification, we observed a substantial amount of microsegregation that had occurred during solidification. Additionally, we observed the presence of carbides, borides and an intermetallic phase on the grain boundaries. All experimental observations point to the cracks being solidification cracks (and not, e.g., liqueation cracks). Cracking mostly occurs on high-angle grain boundaries, in accordance with theories on liquid film stability during solidification. APT also reveals segregation of various elements to the grain boundaries that presumably additionally stabilize the liquid films to low temperatures, thus enabling crack formation during solidification. Scheil-type simulations predict that the solidus temperature of the alloy can be increased substantially if small modifications to the alloy compositions are made. Experiments with accordingly modified alloy powders show that indeed crack-free specimens can be obtained.

(L1 oral) **Numerical investigation of the columnar-to-equiaxed transition using a 2D needle network model**

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The columnar to equiaxed transition (CET) is a morphological transition occurring in casting of metallic alloys. Because of its great technological relevance, this transition has been extensively studied during the past decades. Despite incorporating the relevant physical ingredients, previous analytical and numerical approaches rely on strong assumptions, in particular: (i) the columnar front is assumed to grow at an undercooling predicted by the Ivantsov solution; (ii) the growth of equiaxed grains is assumed to follow a stationary state regime predicted by the Ivantsov solution; (iii) the CET is assumed to occur when the equiaxed grains block mechanically the growth of the columnar front. We test these assumptions with a recently developped needle network model [Tourret, Karma, Acta Mater. 61, pp. 6474-6491, 2013]. This model rigorously treats the diffusive interactions between higher order branches of hierarchical dendritic structures, and describes both transient and steady-state growth regimes of those branches. In order to study the CET, it has been extended to account for the nucleation of new grains and the growth of dendrites with various orientations. We show that assumption (i) is only approximately verified and that the equiaxed grains do not follow the Ivantsov steady-state growth. We also show that for low inoculant concentrations, growth competition becomes a prevalent mechanism and assumption (iii) becomes an oversimplification.

(L2 invited) **Multiscale modelling of hot-tearing**

M Rappaz

EPFL, Switzerland

Hot-tearing and shrinkage microporosity, two major defects of casting and welding processes, are both a result of a lack of liquid feeding within the mushy zone. But hot tearing has the further complexity that it is induced by tensile/shear strains rather than by solidification shrinkage. Being intergranular in nature, hot tearing is clearly linked with the grain structure, and more specifically with the distribution of remaining intergranular liquid films. Over the past fifteen years, understanding and modeling of hot tearing has made substantial progress thanks to a multiscale-multiphase approach. Using MD and multi-phase field modelling, the coalescence/bridging of two solidifying grains (i.e., the reverse of grain boundary wetting) has been shown to play a critical role at the atomistic scale of diffuse solid-liquid interfaces. At the macroscopic scale, the mechanical behaviour of the mushy zone and the critical temperature at which tensile coherency occurs has been approached by mechanical tests, in situ observations and finite element modelling. At the intermediate scale, a granular model of solidification has been developed specifically to account for all of these phenomena: it combines a solidification model, coalescence of grain boundaries, mechanical behaviour of the coherent solid, fluid flow in the remaining liquid network and a defect prediction criterion. Its results have been compared with in situ X-ray microtomography tensile testing observations. This presentation will review such recent developments but also highlight the improvements that still need to be made in this complex topic.

(L2 oral) **Upscaling from mesoscopic to macroscopic solidification models by volume averaging**

M Založnik[1], Y Souhar[1], C Beckermann[2] and H Combeau[1]

[1]Institut Jean Lamour, France, [2]University of Iowa, USA

The mesoscopic solidification model is based on a simplified representation of dendritic structures by their envelopes. It provides quantitative predictions of dendritic growth over a wide range of solidification conditions. Because of its low computational cost compared to microscopic (e.g., phase-field) methods, parametric studies can be performed on a scale that corresponds to the Representative Elementary Volume (REV) used in deriving volume-averaged macroscopic models of solidification processes. In the present study, the mesoscopic model is applied to dendritic solidification of up to 100 interacting equiaxed grains. The results are averaged over the volume containing the grains and then used to obtain constitutive relations for macroscopic models. We present relations for the specific surface area of the grain envelopes and the solute diffusion length from the grains into the extra-dendritic liquid. It is shown that the present computational upscaling approach allows for improved constitutive relations to be obtained.

(L2 oral) **Multiscale modelling of dendritic microstructure**

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The dendritic microstructure forming upon solidification from the melt is of prime importance for the production of materials. For most metallic alloys, it defines the initial morphology of the solid phase to work with upon further processing steps. This is true for Fe, Al, Cu, Mg, Ni, … used as base chemical elements in many manufactured products.

Modeling of dendritic growth has long been a subject of investigation. First developed at the scale of the interface dynamics using mathematical theories, it was then extended to numerical studies at all scale. Modeling of dendritic growth nowadays involves the phase field method at a microscopic scale and various grain envelope methods at mesoscopic scales for integration with multiphase continuum mechanics solvers designed to deal with the macroscopic scale of the casting processes.

This presentation will give an overview of the modeling methods and illustrate developments conducted with the goal to integrate information from the growth kinetics of solid/liquid interface up to heat and mass exchanges taking place at the scale of the cast product. Examples will be provided dealing with processing of limited melt regions or liquid pools as they provide an easier framework for reaching multiscale modeling. For instance, this could include dedicated laboratory experiments with possible in-situ diagnostics and/or welding and additive manufacturing. Current efforts for upscaling models will also be reported.

(L2 oral) **Mesoscopic envelope model and phase field simulations of columnar and equiaxed dendritic growth**

A Viardin[1], M Založnik[2], Y Souhar[2], M Apel[1] and H Combeau[2]

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Integrated computational materials engineering (ICME) aims at predicting the link between the process conditions and the final mechanical properties of the product. Multiscale modeling of solidification patterns is crucial in an ICME methodology of casting. Macroscopic modeling at the process scale, widely used in the industry, lacks an accurate representation of the microstructure. Direct modeling of microstructures is possible with phase field methods, which can accurately predict the strongly coupled phenomena of microstructure formation. Phase field methods are well developed and widely applied, however, due to the calculation time they remain limited to scales of a few grains. The mesoscopic envelope model of dendritic solidification can describe microstructure patterns on the scale of up to 100 dendritic grains. It can thus provide a link between the microstructure and the process scale. In the mesoscopic envelope model, the shape of the dendritic structure is approximated by its envelope. The growth of the envelope is given by analytical models that give the growth velocity as a function of the undercooling of the liquid ahead of the envelope. We present a comparison of mesoscopic and phase field simulations of dendritic solidification in alloys. The objective is to validate mesoscopic simulations of β(Ti) dendrite growth during directional solidification of the binary alloy Ti-45at.%Al under the influence of natural convection in hypergravity. In a first stage, comparisons are performed for columnar and equiaxed dendritic solidification under the influence of diffusive interactions between grains. In a second stage, predictions of the interaction of microstructure growth and fluid flow.

(L2 oral) **Multi-scale modeling of dendritic solidification and the effect of convection on microstructure selection in alloys**

D Tourret[1], Y Song[2], S D Imhoff[1], J W Gibbs[1], A J Clarke[1] and A Karma[2]

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Solidification dendrites are a prime example of a pattern emerging from mechanisms over a wide range of length and time scales. For example, microscopic interfacial effects interact with mass and heat transport at a much larger scale. This transport can be diffusive, but in the presence of gravity, solute and temperature gradients induce significant buoyant liquid motion. We present examples of scale-bridging modelling tools for dendritic solidification, in the context of gravity-induced convection. Our modelling developments are guided by in situ x-ray imaging of tin-bismuth and aluminum-based alloys.

Theoretical developments in phase-field modelling, such as the thin-interface limit, have allowed for quantitative calculations using a diffuse interface much wider than the physical solid-liquid interface, which permits a much coarser numerical discretization. Massively parallel hardware, e.g. Graphic Processing Units, also enables simulations at experimentally relevant length and time scales. Here we present examples of such simulations, coupled with a simple boundary-layer approach to explore convection, and explain microstructural selection trends like the experimentally observed and unexpected increase in primary dendritic spacing with growth velocity in an aluminum-copper alloy during directional solidification.

Additionally, we illustrate a modelling approach designed for dendritic growth with a large separation of scales between dendritic patterns and heat and mass transport. This method quantitatively reproduces phase-field results and experimental measurements in the diffusive regime. Preliminary results of this method, coupled with convective transport in the liquid, are also presented.

(L3 invited) **Crystal-melt interfacial fields: Determinism in pattern dynamics**

M Glicksman

Florida Institute of Technology, USA

Centimeter-long needle crystals melt self-similarly in microgravity, then suddenly exhibit spheroidization when melting reduces their size below 5mm. That surprising shape change observation was investigated theoretically by using the Reynolds transport theorem. Leibniz-Reynolds analysis shows that capillary-mediated energy fields accelerate interface speed during melting and slows it during growth. Conversely, where the field removes energy from an interface, the speed slows during melting and accelerates during growth. Autogenous interface speed modulations reverse direction at 'Laplace point' locations where the energy release itself changes sign. Countervailing modulations on morphologically unstable interfaces can result in inflection and 'curling', which promote branching, forking, invagination, and pattern complexity. Such deterministic interface patterns are already included with phase field and other thermodynamically consistent numerical methods, which confirm quantitatively that deterministic perturbations initiate precisely at the 'Laplace points' of the thermodynamic bias field. A fundamental discovery exposed using field theory is that classic Stefan interface balances–long used in continuum crystal growth theories–remains valid only at macroscopic scales. At smaller mesoscopic scales (10^{-7}–10^{-3} m), where most diffusion-limited microstructure patterns develop, capillary-mediated energy redistribution, per the Reynolds theorem, must also be included. Even persistent interfacial defects, such as stationary grain boundary grooves, conventionally considered as merely static features will be shown to support active capillary-driven energy fields, the divergence of which induces weak interface cooling that guides pattern formation when the interface is unstable. Finally, the relative roles of noise and capillary-mediated perturbations will be discussed.

(L3 oral) **Simulating rapid solidification by a self-consistent sharp-interface model**

K Reuther and M Rettenmayr

Friedrich Schiller University Jena, Germany

Using a highly self-consistent approach, a refined variant of the non-equilibrium solidification model for rapid solidification proposed by Hillert, Rettenmayr [Acta Mat. 51 (2003) 2803-2809] and Buchmann [J. Cryst. Growth 310 (2008), 4623-4627] is implemented for the simulation of one-dimensional rapid solidification of a binary alloy. The model results in three equations coupling the interface velocity and the interfacial concentration at either side of the interface: A mass balance and two equations coupling the interface velocity to the free energy of the alloy.

Based on an implicit time-forward integrating Finite Difference (FD) solver for solute diffusion, the self-consistent approach requires the continuous adaption of the FD node spacing and the time step. The solver is coupled directly to the thermodynamic model via an additional mass balance equation including both the interfacial concentrations and the velocity. As the interface is defined to always reside on an FD node, grid spacing and time step are also coupled by the interface velocity by a fifth equation.

Each time step therefore involves the simultaneous numerical solution of five coupled equations, three of which are nonlinear. The presentation will feature the basic numerical approach towards solving this system of equations, as well as exemplary results for the rapid solidification of the model alloy Al-0.2at%Sn at different temperatures.

(L3 oral) **Crystallographic effects on lamellar eutectic growth patterns**

S Akamatsu, S Bottin-Rousseau and G Faivre

CNRS - UPMC, France

We report on experimental and numerical results on the formation of lamellar microstructures in directionally solidified eutectic alloys that present special orientation relationships (ORs) between the two solid phases (α and β). In such alloys (e.g., Al_2Cu), lamellar eutectic microstructures can grow with a large, eutectic-grain dependent incination (or tilt) with respect to the growth axis. This effect is driven by the anisotropy of the free energy of the α-β interphase boundaries in the solid, which intervenes in the local-equilibrium condition at solid(α)-solid(β)-liquid trijunctions. On the basis of real-time experimental observations, an approximate theory has been proposed, which formalizes this crystallographic effect. In a given eutectic grain, the relative orientation of the α and β crystals is fixed, but the inclination of the α-β boundary can vary. The theory predicts the steady-state lamellar-tilt angle θ_t as a function of the orientation angle $_{\theta R}$ of the eutectic grain with respect to the growth axis. We performed (2d) numerical simulations of tilted lamellar growth patterns by implementing various anisotropy functions of the interphase boundary. The numerical θ_t-vs-θ_R results confirm the general validity of the theoretical proposition. In particular, they shed new light on the dynamic "locking" of eutectic lamellae onto low-energy planes in special-OR eutectic grains. For clarity, we have first considered a generic, symmetric eutectic alloy. Numerical simulations using more realistic alloy constants (asymmetric phase diagram) and various growth parameters (thermal gradient) will also be presented.

(L3 oral) **Theoretical and numerical study of eutectic growth kinetics of NiZr-NiZr2 alloy at low undercoolings**

S Nani Enugala, K Ankit and B Nestler

IAM-CMS, Karlsruhe Institute of Technology, Germany

The Jackson-Hunt's (JH) analysis of eutectic growth kinetics is a standard theory for evaluating the local temperature conditions of experimental microstructures as well as for benchmarking the simulated growth kinetics. Given the assumptions invoked to simplify the JH theory, a major one among which being that of planar solidification front, occasional deviations observed in numerical studies do not necessarily point towards computational under-performance. In this study, we look at one such system and analyze the role played by the flat interface assumption in such a deviation.

First, we simulate the lamellar growth of NiZr-NiZr2 eutectic alloys using a CALPHAD-coupled multiphase-field model based on grand chemical potential formulation. We observe that the morphology of the solidification front is far from being planar and the growth rate versus lamellar spacing plot shows large deviations from the existing JH theory. In view of this discrepancy, we extend the JH analysis by accounting for the curvature of the solid-liquid interface profiles using approximate methods and fourier-like series representations. The importance of this newly developed, curvature-informed JH formulation is realized by a superior compliance between the extended theory and simulated growth kineitcs.

(L3 oral) **Transition path sampling simulations of nucleation during solidification in nickel**

G Diaz Leines, R Drautz and J Rogal

Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, Germany

The initial nucleation of the crystalline phase within the melt is a crucial stage during solid- liquid phase transformations in metal alloys. An accurate modelling of the crystal nucleation on the atomistic level remains, however, very challenging due to the extended timescales of the process.

Here we employ an advanced computational method, transition path sampling (TPS), to elucidate the nucleation mechanism during solidification in nickel. We initially focus on homogeneous nucleation as a function of undercooling. The temperature dependence of the free energy barriers and rate constants that we obtain with TPS is consistent with the predictions of classical nucleation theory (CNT) and experiments. As a second step, we extend our study by including small Ni-clusters as seeds during heterogeneous nucleation. The analysis of the transition path ensemble (TPE) reveals the presence of clusters that consist of fcc and hcp coordinated atoms surrounded by a cloud of prestructured liquid. Furthermore, our simulations show predominantly nonspherical shapes of the nuclei at different undercoolings.

The computation of the TPE also allows a direct evaluation of order parameters to characterize the nucleation mechanisms. We have identified order parameters based on the nuclei local structure and shape as relevant descriptors of the processes. Such results provide valuable atomistic insight into the nucleation mechanisms in metals. In particular, our comparison of heterogeneous and homogeneous nucleation can contribute to the improvement and validation of thermodynamic models like CNT. Moreover, the dynamical information that we obtain can be directly connected to mesoscale models like phase field.

(L4 invited) **Solidification in 4D: from Dendrites to Eutectics**

P Voorhees[1], A Shahani[1], J Gibbs[2], A Mohan[3], B Gulsoy[1], X Xiao[4], C Bouman[3] and M DeGraef[5]

[1]Northwestern University, USA, [2]Los Alamos National Laboratory, USA, [3]Purdue University, USA, [4]Argonne National Laboratory, USA, [5]Carnegie Mellon University, USA

With the advent of high-energy x-ray sources and the development of iterative reconstruction methods, it is now possible to follow solidification processes in three dimensions and as a function of time. The ability to observe and quantify the solidification process in metals on sub-second time scales and micron spatial scales in three dimensions provide fundamentally new insights into this complex phase transformation. For example, measurements of the morphology of Al dendrites growing into an Al-Cu melt show doublon-like side branch evolution. We have also examined the growth of primary Si particles in Al-Si alloys, as well as the growth of the Al-Ge irregular eutectic. We find that twin defects play an essential role in the growth of the primary Si phase from an Al-Si liquid. The Al-Ge eutectic, which consists of a Ge plate-like phase and an isotropic Al phase, grows in cooperative manner as in non-faceted eutectics but with defects that play a critical role in the development of structure. For example, the eutectic propagates in a direction that is perpendicular to slow-growth direction of the Ge plates via the growth of the Al phase through holes in the Ge plates.

(L4 oral) **Critical role of crystal orientation in the large-scale long-time spatiotemporal evolution of array patterns in directional solidification**

A Karma and Y Song

Northeastern University, USA

We use phase-field simulations to investigate the formation of cellular/dendritic array structures during directional solidification of binary alloys in the common situation where the principal crystal axis makes a small angle with respect to the axis of the temperature gradient. The simulations focus on characterizing the large-scale and long-time evolution of the primary spacing in a thin-sample geometry where the array structure is quasi-one-dimensional. The results reveal that a small misorientation induces a slow spatiotemporal evolution of the array spacing towards a stationary, albeit spatially non-uniform, spacing distribution. We derive a nonlinear advection-diffusion equation to predict the large evolution of the primary spacing and the final spacing distribution. This equation gives predictions in very good quantitative agreement with phase-field simulations. Furthermore, it provides a unified theoretical framework to understand the large-scale evolution of the primary spacing in terms of local growth laws and geometrically imposed boundary sources and sinks of cells/dendrites.

(L4 oral) **Phase-field simulations and geometrical analysis of cellular solidification fronts**

M Plapp

CNRS/Ecole Polytechnique, France

We study the structure and dynamics of cellular solidification fronts that are produced during the directional solidification of dilute binary alloys. A quantitative phase-field model in conjunction with multi-scale simulation methods makes it possible to simulate arrays with ten to twenty cells on time scales that are long enough to allow for a significant reorganization of the array. The geometry of the complex two-phase structure (mushy zone) is analyzed in detail. Quantities such as the fraction of solid and liquid as a function of depth, the connectivity of the two phases, the average spacing between cells and their neighborhood relationships, and the orientations of the interfaces are extracted and studied as a function of the processing conditions. The global stability of the array is also investigated. We find a transition from stable arrays at high values of the crystalline anisotropy to unsteady arrays that continuously exhibit tip splitting and cell elimination events at low anisotropy. These findings are compared to available experimental data and phase-field simulations by other groups.

(L4 oral) **Mushy zone solidification and temperature gradient zone melting**

G Boussinot and M Apel

ACCESS, Germany

The solidification paths in most industrial alloys usually involve dendritic growth leaving a complex mushy zone behind the growth front. While the dendritic growth is well documented since alerady a long time, the solidification of the mushy zone has recently received an increasing attention due to the development of in-situ techniques using X-rays. In particular, it has been pointed out that the Temperature Gradient Zone Melting (TGZM) process is a key ingredient in understanding the route to equilibrium of the mushy zone in a directionally solidified alloy.

We performed phase-field simulations of the directional solidification of an Al-Cu alloy, followed by the mushy zone solidification in a static temperature gradient. Our simulations allow us not only to compare with available experimental data, but also to go beyond the experimental accuracy. Especially, we study in details the micro-segregation pattern in the solid, and we analyze the role of TGZM in the development of this pattern.

(L4 oral) **Coupling CALPHAD to phase-field modeling for prediction of microstructure evolution during solidification**

J McKeown, A Perron, J-L Fattebert, J Roehling and P Turchi

Lawrence Livermore National Laboratory, USA

The coupling of phase-field modeling (PFM) to physical databases that include known thermodynamic and kinetic properties is important for realistic parameterization of these models and, in the case of solidification processes, insight to microstructure evolution. Our approach has focused on a combination of thermodynamic and kinetic simulations within the CALPHAD methodology with PFM developed at LLNL to simulate solidification in metallic alloys across a broad range from equilibrium to far-from-equilibrium conditions. A goal of these efforts is development of a tool to predict microstructure evolution under conditions encountered during laser-based additive manufacturing (AM). Modeling successes and challenges—from the initially diffusion-controlled to the diffusionless regimes of the liquid-solid phase transformations—will be discussed and compared with experimental data. Experiments consist of laser surface melting and re-solidification in bulk alloys and *in situ* laser melting and rapid solidification in thin-film alloys. The latter approach, conducted in the dynamic transmission electron microscope (DTEM), permits time-resolved measurements of solidification kinetics and monitoring of the solid-liquid interface and overall microstructure evolution during rapid solidification.

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Work at LLNL was funded by the Laboratory Directed Research and Development Program under project tracking code 15-ERD-006.

(P2.51) **Experimental investigation and thermodynamic modeling of the NiAl-Cr-Mo system**

J Peng[1], P Franke[1], D Manara[2], T Watkins[2], R Konings[2] and H Seifert[1]

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The intermetallic compound NiAl with B2 structure received much attention because of its outstanding physical and chemical properties, compared to Ni-based superalloys. However, its room temperature brittleness and reduced high temperature creep resistance hinder its application as a high temperature structural material. These disadvantages can be overcome by manufacturing an in-situ composite with NiAl matrix strengthening with embedded refractory metals, such as Cr, Mo, by directional solidification of alloys with eutectic composition. In the present work, experimental investigation and thermodynamic modeling of the NiAl-Cr-Mo system are presented in order to support the selection of alloys for directional solidification, microstructure modeling and thermodynamic modeling of higher order systems.

Reliable databases of the sub-systems are the foundation to establish a reliable database of the NiAl-Cr-Mo system. In this work, the liquidus and solidus temperatures of the NiAl-Mo section were measured by a laser heating experiment and a new optimization for the Al-Mo-Ni system was provided where the drawbacks in the previous works were corrected. The Al-Ni-Cr database from literature was modified by considering the contribution of the compound energy of vacancies and re-optimizing the liquid phase. Necessary evaluation for the thermodynamic descriptions of the Al-Cr-Mo and Cr-Mo-Ni systems was carried out. Further, these databases were merged. The optimization for the NiAl-Cr-Mo system focused on the eutectic equilibria between the liquid, NiAl (B2) and the (Cr, Mo) (A2) phases. The calculated eutectic trough of the NiAl-Cr-Mo system agreed well with our experimental results and literature data.

(P2.52) **Upscaling the microscopic crystal growth dynamics in snow**

Q Krol and H Löwe

WSL Institute for Snow and Avalanche Research SLF, Switzerland

Macroscopic properties of heterogeneous, multi-phase materials can be conveniently characterized in terms of spatial correlation functions. If microstructures evolve under thermodynamic forcing, a consistent upscaling scheme requires including the dynamics of the correlation functions as microstructural characteristics. This scenario is of key importance for snow on earth where microscopic crystal growth processes respond quickly to applied temperatures and temperature gradients on a centimeter scale. We address this problem by considering the Taylor expansion of the two-point correlation function, which involves the volume-averaged geometrical parameters such as relative density, specific surface area and Gaussian as well as squared mean curvature. We extend a previously derived, geometrical upscaling framework to obtain a system of coupled differential equations for all parameters emerging in the correlation function. The system must be equipped with a growth law, i.e., an expression for the interface velocity, as a closure for the evolution equations. In the absence of suitable models for the growth law, we exploit experimental data obtained from micro-computed tomography. By using VTK-based image analysis techniques on time-lapse experiments of snow, we can track the growing ice-air interface. This enables us to assess the relevance of individual terms in the coupled system of equations providing a basis for systematic improvements of common snowpack models.

(P2.53) **Application of directional solidification techniques to thermoelectric Bi2Te3-In2Te3**

D Liu and M Rettenmayr

Friedrich Schiller University Jena, Germany

Advanced solidification techniques are applied to control microstructure and hence properties in a novel functional material. In the present work, thermoelectric (Bi, In)$_2$Te$_3$ is used. Mushy zone resolidification in a steep temperature gradient was first used to accurately determine the liquidus, and solidus lines in the phase diagram. A specially adapted zone melting technique with seeding was then developed to prepare a (Bi, In)$_2$Te$_3$ solid solution, with defined crystal orientation and enhanced chemical homogeneity along the entire grown crystal. These features allow quantitative control of meso- and nanoscaled precipitation structures and the formation of an aligned alternating Bi$_2$Te$_3$/In$_2$Te$_3$ layer structure, resulting in a composite material with enhanced thermoelectric properties along the growth/layer orientation, The materials properties are explained using analytical equations (mixture rules) for the two-phase structures. Deviations of the experimental results give hints to specific processes occurring at the internal interfaces.

(P2.54) **Meshless front tracking - a novel simulation method for anisotropy sensitive solidification problems**

K Reuther[1], B Sarler[2] and M Rettenmayr[1]

[1]Friedrich Schiller University Jena, Germany, [2]University of Nova Gorica, Slovenia

A novel spatially and temporally resolved Meshless Front Tracking method for the simulation of the movement of phase interfaces is presented. Contrary to established simulation methods, the method is not based on a regular mesh with necessarily anisotropic properties, but instead on an isotropic, random set of points ("grid"). It therefore introduces no artificial numerical anisotropy into the simulated interface geometry, allowing the simulation of problems that are sensitive to anisotropic physical entities such as interfacial energy.

The time-forward-integration solver for the governing partial differential equation uses special algorithms for the suppression of the numerical noise induced by the irregular grid. The moving interface is represented by Lagrangian particles moving between the grid points. This allows straightforward coupling of the interface and its mass balance to the diffusion solver as well as a consistently local formulation of the problem, which in turn allows massively parallel calculations.

In the presentation, basic concepts of the Meshless Front Tracking method are introduced and its capabilities are demonstrated using an exemplary simulation of early stages of dendritic solidification in a binary alloy.

(P2.55) **In-situ observation of pattern formation in In-Bi-Sn eutectic system in quasi-2D samples**

S Mohagheghi and M Ş Kaya

Koç University, Turkey

Solidification microstructure is the trace left in solid, imprinted by a propagating solid/liquid interface. In a well-controlled experimental condition, the micro-scale pattern, formed during unidirectional solidification of a eutectic alloy with isotropic interfaces, exhibits self-organized array of lamellar or rod structures in a quite large scale. In a 2D three-phased system, one can expect diverse phase configurations; for instance, ABC, ABAC or ABABC repeating units, where A, B, and C are the crystalline phases.

In this work, we present a study on the in-situ observation of the microstructure formed during directional solidification of In-Bi-Sn eutectic system. Quasi-2D samples (13 – 100 μm) at eutectic composition were directionally solidified using a horizontal Bridgman setup. The dynamics of microstructure formation were examined in real time using computer controlled high resolution motor and a special optical microscopy system, which enables observation of solidification front from top and bottom simultaneously. We first map the morphological stability diagram for the ABAC pattern and characterize the instabilities occurring beyond the limits of stability in this system. We will explain a novel mechanism called "phase exchange", through which an ABAC pattern destroyed by instabilities is able to recover itself. Finally, we will report a new microstructure, which we believe is formed due to high anisotropy of the solid/solid interfacial energy.

(P2.56) **Comparison of 2D multi-scale dendrite needle network modelling to x-ray radiography of multiple equiaxed grain growth in grain-refined Al-3.5wt.-%Ni**

L Sturz and A Theofilatos

Access e.V., Germany

The aim of this work is to investigate multiple dendritic equiaxed grain formation during directional solidification of grain-refined Al-3.5wt.-%Ni under a range of different solidification conditions. This is achieved by comparing the results of in-situ x-ray radiographic experiments involving thin samples (as reported in the literature) to the results of 2D multi-scale dendrite needle network (DNN) modelling covering the essential experimental length scale. The model takes into account heterogeneous nucleation, branched dendritic growth and solutal interaction between branches and multiple equiaxed grains. The decrease in equivalent circular diameter of the steady-state average grain size with pulling velocity, as observed in the Bridgman-type experiments, is well captured by the modelling results, and likewise the ratio of activated nucleation seeds. Using experimentally estimated nucleation parameters in the modeling, a log normal nucleation undercooling distribution provided slightly but not significantly better agreement with experiments than a Gaussian distribution, with remaining absolute differences in the equivalent circular diameter of up to 31%. Thus, even with the 2D modelling of an essentially 3D experiment, fairly good agreement is achieved. Moreover, dendrite side-branching in modelling is of minor impact, due to a ratio between solutal diffusion length and equivalent circular diameter inferior to 0.49 under all solidification conditions. Additionally, the computed grain density is only slightly dependent on which unknown dendrite selection parameter σ^* over a wider range is selected.

(P2.57) **Development of solidification models for molten salt coolants**

M T Retamales[1], P Rubiolo[1] and O Doche[2]

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Due to their exceptional heat capacity and stability in high temperature and irradiation environments molten salts have been proposed as coolants in the nuclear reactors (e.g. Molten Salt Reactor) and also in solar concentration applications. Nevertheless, their high melting point poses some technical challenges. For example, during some normal operation and accidental scenarios, unwanted solidification may occur in the molten salt circuit under a strong external convection. Consequently, an adequate design of these systems requires a better understanding of the dynamics the solidification process and the resulting solid phase microstructure together with accurate numerical models.

In this work a two levels approach is proposed for studying the multi-scale solidification phenomena for a molten salt coolant. First, a one domain approach macro-mode model is used for studying the evolution of the solid-liquid interface assuming the fraction of solid to be linearly dependent on the undercooling temperature. Then, a meso-scale phase field model was developed for understanding the mechanical and morphological properties of the solid micro-structure. Afterwards, the coupling of both models by equating the growth velocity of the solid-liquid interface is presented. The comparison of the results of the proposed model against data available in the literature shows a very good agreement. Finally, the experiments being designed for validating the models will be presented.

(P2.58) **In-situ X-ray investigation of dendritic growth kinetics and solutal field interaction of an Al-Ge alloy in comparison with DNN-modeling**

M Becker[1], L Sturz[2], A Theofilatos[2], S Klein[1] and F Kargl[1]

[1]Deutsches Zentrum für Luft- und Raumfahrt, Germany, [2]Access e.V., Germany

Equiaxed dendrites are a common solidification growth form in metal alloy castings. The growth process is mainly governed by heat and solute diffusion and at a later growth stage particularly by the interaction of adjacent grains. In-situ X-ray imaging is our method of choice to investigate equiaxed grain formation in thin horizontally aligned Al-Ge samples. Our main objective is to analyse the interactive relationship between structure formation and solutal field evolution and to compare our experimental findings with growth models. The thin sample geometry and especially the horizontal sample alignment result in preferentially near diffusive solidification conditions since buoyancy- and gravity-driven melt flows are minimized. Calibration measurements of samples of known compositions and thickness are used to determine absolute compositions in the liquid during the ongoing solidification. Thus quantitative comparison with dendrite growth models is possible.

We compare the microstructure and the solutal compositions of the experiment to the results of a 2D multi-scale dendrite needle network (DNN) model on the experimental length scale that takes into account the solutal interaction of multiple equiaxed dendrites. In a first attempt the idealized model uses the experimentally determined nucleation events to calculate dendrite evolution and solutal concentration profiles. Qualitatively the model reproduces the solutal concentrations of the experiment quite well.

Additionally, the measured concentrations are applied to the McFadden-Brown growth model (an extension of the Lipton-Glicksman-Kurz sharp interface model which allows for increased solute levels) resulting in comparable modeled and measured dendrite tip velocities.

(P2.59) **Macroscale modelling of Bridgman furnace solidification for the prediction of texture evolution and columnar to equiaxed transition**

R P Mooney[1], S Battaglioli[1], S McFadden[2] and A Robinson[1]

[1]Trinity College Dublin, Ireland, [2]University of Ulster, Ireland

Bridgman furnaces are commonly used in solidification research owing to their convenience when setting the desired solidification parameters, specifically, the nominal temperature gradient and nominal growth rate. The work outlined here describes the development of two macroscopic models for the prediction of texture evolution in Bridgman furnace experiments that use cylindrical shaped samples. The first model employs a 1-dimensional axisymmetric thermal model (suitable for small sample diameters) with columnar mush front tracking; equiaxed growth is analytically modelled using the Avrami's extended volume concept. The second model employs a 2-dimensional axisymmetric thermal model (suitable for small and large sample diameters), also with columnar mush front tracking; in this model an indirect method of columnar to equiaxed transition prediction (Equiaxed Index) is employed. Both models have been developed as part of the European Space Agency research projects: GRADECET (Gravity Dependence of Columnar to Equiaxed Transition in Gamma Ti-Al Alloys) and CETSOL (Columnar to Equiaxed Transition in Solidification Processing), for the purposes model validation and enlightenment of planned future experiments.

(P2.60) **Embedding a microstructure model in a continuum scale casting code**

J Gibbs, N Carlson, S Imhoff, P Gibbs, D Tourret, P Papin, R Forsyth, F Merrill and A Clarke

Los Alamos National Laboratory, USA

Casting modelling at the macro-scale has a long and successful history, but the ability to predict microstructure from these models is difficult, due to the large separation in scale between microstructural features and larger-scale phenomena like heat transfer and fluid flow. Here we present a method of bridging these length scales by embedding a microstructure formation model into a continuum-scale casting code to predict solidification morphology and as-solidified cellular or dendritic spacings (i.e., microstructural characteristics). Model validation was done by casting a tin-bismuth alloy into a wedge-shaped mold to produce a wide variety of solidification conditions and a range of microstructural characteristics. Characterization of the sample was done by a combination of location-specific temperature measurements in the casting mold and 800 MeV proton radiography (pRad) to observe the mold heating, alloy melt filling, and cooling behaviours. Post-mortem electron microscopy was also performed to measure dendrite arm spacing's. This experimental and model comparison shows the promise of this type of embedded model in predicting dendritic solidification behaviour.

(P2.61) **Eutectic growth in two-phase multicomponent alloys**

O Senninger[1] and P Voorhees[2]

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Most of fundamental studies on the formation of self-architectured composite materials during solidificaiton of eutectic alloys have been carried out by considering binary eutectics. However, industrial eutectic materials usually contain more than two compounds, which makes their solidification, diffusion-controlled dynamics much more complex, and still poorly understood. We present a theoretical study of two-phase growth in multicomponent eutectic alloys. Our analysis uses the same hypotheses as the well-known Jackson-Hunt theory of regular eutectics. The thermodynamic parameters involved in the theory are derived from the Gibbs free energies of the three phases (the liquid and the two solids) in coexistence. This makes it possible to compute the parameters of interest with CALPHAD tools. A model is derived for ternary alloys from this general theory, without oversimplifying assumptions (e.g., equal diffusivity for all compounds) that were used in previous work. Interestingly, we find that a small addition of a ternary alloying element with a much smaller diffusion coefficient than the other ones can significantly modify the characteristic interpahse spacing of the microstructure, as compared to binary eutectic alloy of reference.

Symposium M

(M1 invited) **Local strain measurements during in situ TEM deformation with nanobeam electron diffraction**

A Minor[1], C Gammer[2], Y Deng[3], C Ophus[4], P Ercius[4] and J Ciston[4]

[1]University of California Berkeley, USA, [2]Erich Schmid Institute of Materials Science, Austria, [3]Nanjing University, China, [4] Lawrence Berkeley National Laboratory, USA

This talk will highlight recent advances with in situ Transmission Electron Microscopy (TEM) nanomechanical testing techniques utilizing scanning nanobeam electron diffraction techniques to map local strain [1,2]. In addition to providing insight into the strength of small-volumes, measuring the evolution of strain during plastic deformation is of great importance for correlating the defect structure with material properties. With the advent of fast direct electron detectors and controlled *in situ* mechanical testing techniques, local strain mapping can be carried out during in-situ deformation in a TEM with the precision of a few nanometers without stopping the experiment. The technique of local strain mapping consists of recording large multidimensional data sets of nanodiffraction patterns before, during and after the experiment. This dataset can then be reconstructed to form a time-dependent local strain-map with sufficient resolution to measure the transient strains occurring around individual defects. We have recently used this technique to probe the evolution of strain in metals during *in situ* tension and nanoindentation tests, and in ferroelectric materials during bending and compression. The combined results demonstrate that local strain measurements can provide enhanced information (see Figure 1) during *in situ* mechanical testing with a spatial resolution varying from many nanometers down to atomic resolution.

[1] C. Gammer, et. al., *Ultramicroscopy,* 155, p. 1-10 (2015)
[2] V.B. Ozdol, et. al., *Applied Physics Letters*, 106, 253107 (2015)

(M1 oral) **Plasticity of Olivine Mg2SiO4: Insights from nanomechanical experiments and atomistic calculations**

S Mahendran[1], P Carrez[1], C Bolinger[2], H Idrissi[3] and P Cordier`

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It is now accepted that thermal convection of Earth mantle is constrained in its upper part by the plastic properties of olivine (a silicate of composition (Mg,Fe)2SiO4). In this study, we revisit dislocation plasticity of Mg2SiO4 single crystal by combining small scale in-situ deformation experiments and atomistic calculations of dislocation core properties. We consider two typical types of dislocations characterized by either [100] or [001] Burgers vectors. In-situ TEM nanomechanical testings are used to infer the dependence of critical resolved shear stress on temperature. The fundamental understanding of how dislocation glide motion is influenced by the pressure-temperature conditions is investigated by dislocation core properties calculations using empirical potentials combining coulombic interactions and core-shell model for oxygen atoms. We will show that atomistic calculations, consistent with experimental results can further contribute to elucidate the plastic deformation behavior of olivine in Earth mantle conditions.

(M1 oral) **Dislocations in ferroelectric perovskite $KNbO_3$: Insight from theory and experiment**

P Hirel[1], A F Mark[2], M Castillo-Rodriguez[3], W Sigle[2], M Mrovec[4] and C Elsässer[4]

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Potassium niobate $KNbO_3$ is a lead-free perovskite and a promising candidate to replace lead-containing ferroelectrics related to $PbTiO_3$. This class of materials has a wide range of applications, like ferroelectric random access memories. Yet the reliability of components relies on the control and prediction of functional properties, which can be achieved only with a good knowledge of the properties of defects. In particular, extended defects such as dislocations are known to act as pinning points for domain walls, thus hindering ferroelectric switching.

In this work, dislocations in $KNbO_3$ are investigated by the combined use of atomistic computer simulations and transmission electron microscopy (TEM). The purpose is two-fold: first to establish the relationship between the elementary behavior of dislocations and the macroscopic plastic deformation of the material; and second, to understand the interactions between dislocations and ferroelectric domain walls. Deformation experiments show the predominance of the <110> slip system at all temperatures, in agreement with predictions from atomic-scale calculations. The core structure of dislocations are simulated at the atomic scale, and compared with high-resolution TEM images. Evidence is found for the nucleation of domain walls from dislocations during the phase transitions, consistent with the polarization field around dislocations as determined from atomistic calculations.

[1] P. Hirel et al., Phys. Rev. B 92 (2015) 214101

(M1 oral) **Understanding Atomic Force Microscopy: From atomic to macroscopic scale**

A Shluger and D Gao

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Non-contact Atomic Force Microscopy (NC-AFM) is a powerful method for studying the structure and processes at surfaces with atomic resolution. A sharp tip oscillates with constant amplitude and sophisticated electronics monitors the minute changes in the frequency of tip oscillations as it scans the surface. For achieving atomic resolution, the end of the tip approaches the surfaces as close as 0.2 nm. The operation of NC-AFM includes several length- and time-scales. The strongest interaction is the van der Waals interaction between a macroscopic tip and a sample. Chemical resolution is due to the relatively small variations in the interaction between a nano-tip closest to the surface and different surface atoms. The frequency of tip oscillations is in the range of several hundred kHz, but the scan speed is of the order of one scan-line per 0.1 s, whereas the response of the electronics is in the micro-second regime. These factors affect the ability of NC-AFM to observe dynamic surface processes, such as diffusion, reactions or manipulation of adsorbed molecules. Modelling NC-AFM imaging is vital for interpretation of observed images. We will demonstrate how the quantum mechanical modelling of the chemical interaction is combined with the van der Waals interaction of the macro-tip to correctly represent the tip-surface interaction. This interaction is then fed into the complete model of the NC-AFM electronics (so called Virtual AFM) to model NC-AFM images. The results will be illustrated by comparing theoretical and experimental NC-AFM images of atom manipulation at ionic surfaces.

(M2 invited) **Dislocation and back stress dominated viscoplasticity in freestanding sub-micron Pd et Cu films**

T Pardoen, G Lemoine, M-S Colla, R Vayrette, H Idrissi, H Tummalla, M Fivel, J-P Raskin and L Delannay

Université Catholique de Louvain (UCL), Belgium

Plasticity in nanocrystalline metals, in bulk or thin film form, involves a complex interplay of mechanisms: dislocation nucleation, glide, starvation, recovery and/or accumulation, grain boundary migration and sliding, grain growth and self-diffusion. Depending on grain size, grain morphology, composition, deformation level, loading rate and temperature, one or a combination of these mechanisms can dominate over the others. In a set of studies on nanocrystalline Pd films with 100 to 500 nm thickness, we found that dislocation mediated plasticity was the dominant deformation mechanism even though the mean grain size was 30 nm. Another recent set of results on Cu films, with bimodal grain size distribution, also in the sub-micron range, showed a dominance of dislocation mediated mechanisms as well. In both cases, the films exhibit moderate to high ductility, moderate to high rate sensitivity and significant kinematic hardening. All these results have been obtained using an on chip tests method allowing for clean uniaxial tensile tests under a variety of conditions, involving creep, and amenable to in situ TEM characterization.

After summarizing the key experimental findings, it will be shown that "classical" polycrystal viscoplasticity captures, after parameter identification, all these findings. The essential features of the model involve a grain size distribution to capture back stress and dislocation based viscoplastic law. A single viscoplastic hardening law is sufficient to predict both short term rate effects and long term creep relaxation. The assumptions of the polycrystalline model are assessed by comparison with 3D discrete dislocation dynamics simulations on representative grain aggregates.

(M2 oral) **Micro-fracture testing of Tungsten: Simulation and experiment**

S Weygand[1], N Schmitt[2], T Volz[1], C Bohnert[3] and R Schwaiger[2]

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Tungsten is a very promising structural material for the use in power generation applications. However, its brittleness and high brittle-to-ductile transition, far above room temperature limits its application significantly. Previous studies have shown that the microstructure has a significant influence on the deformation and fracture behavior. In this study, microscale fracture experiments were conducted in combination with finite element simulations with the goal to separate the contributions of plasticity and cracking and develop a procedure to determine the fracture toughness of micro-scale, non-standard specimens.

Free-standing single-crystalline micro-cantilever beams of two different sizes, i.e. width and length of 40 µm and 160 µm compared to 15 µm and 80 µm, respectively, were tested. The specimens were fabricated by micro-electro-discharging machining and focused ion beam (FIB) milling to test different crack systems. After introducing a Chevron notch using FIB, the cantilever beams were loaded using a nanoindenter. Finite element simulations were closely matched with the experiments. In the numerical analysis, the framework of crystal plasticity was used to account for the anisotropic plastic behavior of these single crystals while cohesive zone elements were implemented to describe crack initiation and crack growth. By combining simulation and experiments, we will show that fracture toughness values can be determined based on experimental load-deflection curves of notched microcantilever beams despite the occurrence of plastic deformation. The influence of sample dimensions will be discussed.

(M2 oral) **Dislocation Dynamics simulations and in-situ TEM observations of interactions between dislocations and irradiation induced loops in recrystallized Zircaloy-4**

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CEA, France

A better understanding of the effect of irradiation on the mechanical properties of zirconium alloys is important in nuclear applications. The aim of this present work is to study the elementary mechanisms occurring during post-irradiation deformation of these alloys. Plastic deformation, due to the dislocation glide, is controlled by interactions between dislocations and radiation induced defects which lead to the formation of defect free channels. We report here both an experimental and a numerical study of this mechanism.

The experimental study is based on in-situ tensile tests carried out in a Transmission Electron Microscope (from 25 to 500°C) on recrystallized Zy-4 samples pre-irradiated with Zr^{+} ions. Interactions between dislocation loops and dislocations, gliding either in prismatic or pyramidal planes, have been observed and, in some cases, the incorporation of the loop into the dislocation as a super jog or helical turn occurred. While in-situ TEM observations provide valuable information on the occurrence of such interactions, they fail in retrieving the details of these interactions at the loop scale.

Dislocation Dynamics simulations, using NUMODIS code, are able to describe in detail the interactions at such scale but need inputs such as the dislocation mobility law and appropriate stress level. The simulations are performed in the same geometrical configuration, time scale and stress conditions. The good qualitative and quantitative agreement validates the interaction mechanisms, and opens the door to large scale and realistic simulations that should lead a better understanding of defects free channels formation.

(M2 oral) **The effect of dimensionality and size on the nanoindentation – A combined experimental/computational multiscale study**

S Roy[1], R Gatti[2], B Devincre[2] and D Mordehai[1]

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The strength of metallic specimens strongly depends on dimensionality and size while approaching the sub-micrometer scale. Via nanoindentation experiments on Au thin-film and nanoparticles, we demonstrated that nanoparticles are substantially softer than thin-films of the same height and the smallest nanoparticles are softer than the largest ones [1]. Here we present a combined experimental/computational approach to investigate the dislocation mechanisms governing nanoindentation of particles. Using molecular dynamics (MD) simulations we revealed how dislocations are nucleated beneath the indent and interact with free surfaces. Small nanoparticles exhibit dislocation starvation shortly after nucleating the first dislocations while in the larger a dislocation density is accumulated around the indent. MD simulations are limited in size, so in order to bridge between the scales, discrete dislocation dynamics (DDD) were performed. In DDD simulations we introduced a nucleation criterion inspired by MD simulations and the nanoindentation stress field distribution inside the nanoparticle was calculated with finite element simulations. DDD simulations shown again that dislocations escape at the free surfaces more easily in smaller particles and the plastic zone beneath the indent increases with nanoparticle size. Furthermore when dislocation collinear annihilation occurs in the plastic zone, dislocations are effortlessly driven out of the particle. This starvation feature is associated to particular slip-traces on surfaces. Finally, our multiscale approach captures the underlying dislocation mechanisms controlling the size-effect in nanoindentation and can be used to develop a dislocation-based continuum law for the nanoscale.

[1] D. Mordehai, M. Kazakevich, D. J. Srolovitz, and E. Rabkin. Acta Materialia, 59:2309, 2011

(M2 oral) **Toward the understanding of the brittle to ductile transition at low size in Silicon: Experiments and simulation**

J Godet[1], F Abed El Nabi[1], L Pizzagalli[1], S Brochard[1], C Tromas[1], L Thilly[1], M Texier[2] and O Thomas[2]

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While bulk silicon is brittle at temperatures below 600-700K, the compression of nanopillars has shown that a decrease of the diameter below few hundreds of nanometers could change the silicon behavior from brittle to ductile at room temperature. Nowadays the respective improvements in simulations and experiments allow to investigate the mechanical properties of objects of similar sizes, close to hundreds of nanometers. We have then used both approaches - experiments and simulations – to understand the mechanisms at the origin of cracks and dislocations nucleation in such nanopillars.

Experimentally, nanopillars with diameters of 100 nm are obtained by lithography. They are compressed by a flat punch nano-indentor under controlled-displacement mode at 300K, and analyzed by SEM and HRTEM. In simulation, nanopillars up to 44 nm in diameter and height are investigated under compression and tension in controlled-displacement too.

In compression, both approaches reveal a ductile behavior with similar stress-strain curves, and large shear bands of amorphous silicon along the slip plane. The simulations under tensile load show the nucleation of perfect dislocations from the surface that can lead to cavity opening when they interact [Abed-El-Nabi MSMSE 2015].

We observe that the brittle to ductile transition is controlled by the diameter of the nanopillars, as observed experimentally in compression. The simulations seem to corroborate the fact that the size of the brittle to ductile transition could increase with temperature, as presumed experimentally.

(M3 invited) **Using FFT-based simulations to incorporate local twinning features into Polycrystal Plasticity modeling**

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Twinning is an important deformation mechanism in hexagonal close packed (HCP) materials. Twinning provides large localized shear inside grains, and takes place in sequence, starting with nucleation followed by propagation and growth. Each of the above processes depends on local microstructural and mechanical fluctuations at the atomic, intragranular, and intergranular scales. As a consequence, implementing twinning in Polycrystal Plasticity Models, requires to have a strategy in place for incorporating such local dependence. Here, we do so by linking full-field Fast Fourier Transform (FFT) simulations with the macro-scale effective-medium VPSC model. We use the FFT model for establishing statistical correlations between grain size, neighboring grain orientation, twin stress fields, and backstresses associated with twinning. These statistical correlations are implemented probabilistically in the VPSC model and applied to simulate deformation of Zr and Mg and {10-12} tensile twin activity. The results of this approach allows us to explain and predict the following twinning observations: 1) distribution of twin variants and twin thickness; 2) why small sized grains tend to twin less; 3) why twins in Mg are thicker than twins in Zr; 4) why twins prefer to transmit across grain boundaries with low misorientation. The model predictions are validated with experimental EBSD observations and statistical characterizations. The results clearly show the importance of accounting for these effects in order to explain the observed mechanical response of HCP materials.

(M3 oral) **Multiscale modeling of IN718 superalloy based on micropillar compression and computational homogenization**

J Llorca[1,2], A Cruzado[1], B Gan[1], J Segurado[1,2] and J Molina-Aldareguía[1]

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A multiscale modeling strategy is presented to determine the effective properties of polycrystalline Ni-based superalloys. They are determined by computational homogenization of a representative volume element of the microstructure which was built with the grain size, shape and orientation distributions of the material. The mechanical behavior of each grain was simulated by means of a crystal plasticity model, and the model parameters that dictate the evolution of the CRSS in each slip system (including viscoplastic effects as well self and latent hardening) were obtained from compression tests in micropillars milled from grains of the polycrystal in different orientations suited for single, double (coplanar and non coplanar) and multiple slip. The multiscale model predictions for the strength of wrought IN718 were in good agreement with the experimental results.

(M3 oral) **Lattice strain evolution during biaxial loading of 316L stainless steel cruciform samples using an FE-FFT approach**

M Upadhyay[1], S Van Petegem[1], T Panzner[1], H Van Swygenhoven[1] and R Lebensohn[2]

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In this work, a multi-scale elastic-plastic finite element (FE) and fast Fourier transform (FFT) approach is proposed to study lattice strain evolution in cruciform samples of 316L SS subjected to biaxial loads. At the macroscale, FE simulations predict that the cruciform geometry induces a coupling between applied forces along both cruciform axes and the stresses in the gauge region. For instance, uniaxial loading in the cruciform samples results in a biaxial stress state with a compressive component along the direction normal to the loading direction. As a consequence, computing the stresses in the gauge area as force along a given axis divided by cross-sectional area along that axis, typically done for the ISO standard cruciform geometry, may result in significant errors.

FE simulation predicted stresses are used as macroscopic boundary conditions to drive the mesoscale elasto-viscoplastic FFT model. The combined FE-FFT approach appropriately captures the lattice strain evolution for different applied load ratios for the cruciform samples.

Next, a detailed analyses of the lattice strain evolution during uniaxial and equi-biaxial loading in cruciform samples is performed. Results reveal that the contribution of elastic and plastic anisotropy on the lattice strain evolution depends on the applied stress ratio. Furthermore, this dependence varies significantly for different grain families. This study has led to the development of a biaxial load dependent theoretical formulation of elastic compliance and slip activity in cubic crystals.

(M3 oral) **Quaternion correlation for tracking crystal motions**

Q Shi[1], F Latourte[1], F Hild[2] and S Roux[2]

[1]EDF R&D, France, [2]LMT Cachan, France

During in-situ mechanical tests performed on polycrystalline materials in a scanning electron microscope, the crystal orientation maps may be recorded at different stages of deformation. The present study introduces a novel correlation technique that exploits the crystallographic orientation field, which is obtained from electron backscattered diffraction, as a surface pattern to track crystal motions. Resorting to a quaternion-based formalism and linear quaternion interpolation reveals very convenient to handle crystal symmetry, cost function and orientation extraction. Spatial regularization is provided by a penalty to the deviation of measured displacement fields from being the solution to a homogeneous linearly elastic problem. This procedure allows the displacement to be interpolated within the grains and hence the crystal rotations, both rotation axis and angle, to be estimated from the residual quaternion field.

This technique has been successfully tested on virtual EBSD images generated using crystal plasticity finite element calculations and on experimental data. A root mean square displacement error of the order of 0.3-0.4 pixel and a corresponding rotation error of the order of 0.001 degree are obtained for the first test case. Then the technique is carried out to track grain boundary motions at sub-pixel levels and to measure rotation fields at the grain scale with a real microstructure.

(M4 invited) **Coupling microstructure-sensitive modeling and in situ experiments to improve fatigue life predictions**

M Sangid, S Yeratapally, D Naragani, A Mello and J Rotella

Purdue University, USA

Fatigue remains to be a critical and challenging issue for engineers and scientists. During cyclic loading, the stress state and structure of the material are evolving, which results in a dynamic problem with many variables to consider. Given the vast microstructure variations in structural engineering materials, it poses a problem of how the uncertainty in the microstructure propagates to variability in the fatigue response of the material. Of greater interest to our community, is how do we account for the uncertainty in defect/microstructure distributions within our material in our life predictions and analysis. The focus of this talk will be an overview of research efforts to understand, model, and verify activities for crack nucleation resulting from persistent slip bands. Results from *in situ* fatigue experiments, in the form of (i) concurrent digital image correlation and electron backscatter diffraction and (ii) high energy x-ray diffraction microscopy, are discussed to map strain evolution relative to the materials microstructure. Finally, we note that as a result of fatigue life limitations in gas turbine applications, many components are overdesigned leading to increased weight and lower operating temperatures of the engine. Thus, significant energy efficiency benefits exist with better fatigue life prognosis.

(M4 oral) **Unravelling dislocation collective properties with dislocation dynamics simulations for continuous modelling**

V Verbeke[1], B Devincre[1] and S Sandfeld[2]

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Predicting and understanding the collective evolution of dislocation microstructures under cyclic loads with the resulting mechanical properties is a long-goal of physically based multi-scales modeling. Despite many years of investigations, dislocation patterning is still an unsolved problem and a major issue since heterogeneity in the dislocation density causes strain gradient and therefore kinematic hardening.

Recent studies emphasized the key contribution of short-range dislocation interactions in patterning processes. In multi-slip conditions, forest interactions and junction formation are the main features controlling dislocation storage and the formation of dislocation microstructures with specific crystallographic orientations. In single-slip condition the picture is less direct, but pattering seems to be controlled by collinear annihilations taking places between mobile dislocations and complex dislocation loop debris with collinear superjog, i.e. edge segments in the cross-slip plane. Those annihilations give an explanation for the accumulation of edge dipolar loops and the formation of dislocation bundles and walls in cyclic deformation.

In the present study, precise direction-dependent interaction coefficients accounting for junction strengthening and collinear annihilation are determined from 3D-DD simulations. Such coefficients are thought to be essential parameters for continuous modeling of dislocation dynamics such as CDD or PF simulations since they control the driving forces leading to the formation of dislocation density heterogeneities.

(M4 oral) **Analysis and data mining of discrete dislocation data with the D2C framework**

D Steinberger[1], S Sandfeld[1] and B Devincre[2]

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Understanding the motion and interactions of dislocation is crucial in unravelling the influence of the microstructure on the mechanical behavior of crystalline materials. In recent years several methods were developed to investigate dislocation properties on the micro scale. Discrete Dislocation Dynamics (DDD) are well established, but are limited to relatively small samples and low dislocation densities/strains. Continuous Dislocation Dynamics (CDD) alleviate these drawbacks but have yet to be applied to complex problems where validation of the method via analytical solution is not feasible.

With "D2C" we introduce a framework where discrete dislocation data from DDD or other sources, as e.g. experiments or atomistic simulations, can be used to compute continuum fields describing the dislocation ensemble. The level of detail can be adjusted by the amount and types of fields computed. Besides the validation of CDD via DDD [1] the approach enables the quantitative comparison of different microstructures and loss of information in different continuum dislocation models.

We show how "D2C" in conjunction with ensemble averaging can be applied to 3D DDD simulations of a bicrystal under monotonic and cyclic loading Simulations are compared with respect to their resulting microstructure and stress state near the grain boundary. We investigate which continuous fields are necessary to describe this microstructure faithfully. Finally, we show first results from
analyzing some of the largest existing DDD simulations that exhibit dislocation patterns.

[1] S. Sandfeld and G. Po, Model. Simul. Mater. Sci. Eng. 23.8, 2015

(M4 invited) **Dislocation transfer through twin-boundaries analyzed by x-ray µLaue diffraction**

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The deformation behavior of metallic single crystals is size dependent, as shown by several studies during the last decade. Nevertheless, real structures exhibit different interfaces like grain, twin or phase boundaries. Due to the possibly higher stresses at the micron scale, the poor availability of dislocation sources and the importance of diffusion in small dimensions the mechanical behavior of samples containing interfaces can considerable differ from bulk material.

One remarkable exception is the deformation behavior of coherent S3 (111) twin boundaries, were apparently the twin boundary does not influence the measured stress strain behavior of micron sized compression pillars with respect to its single crystalline counterbodies. This work extends the former in situ scanning electron microcopy study of Imrich (Acta Materialia 2014) by using (i) coherent S3 (111) twin boundaries loaded in different directions and (ii) applies µLaue diffraction in order to investigate the number of piling up dislocations.

During the experiments load, displacement and µLaue diffraction patterns are recorded continuously, and thus, the crystallographic orientation, phase, deviatoric strains and density of geometrically necessary dislocations can be monitored during deformation. The talk will focus on pile-up of dislocations at the boundary, slip transfer mechanisms, storage of dislocations and dislocation networks at the different interfaces. Finally, the results will be compared to the experiments of Jeon and Dehm (Scripta Materialia 2015).

(M5 invited) **Modelling plastic deformation in micro- and nano- samples using the Discrete-Continuum Model**

R Gatti

LEM, UMR 104 CNRS-ONERA, France

Plastic deformation of crystalline materials is the result of the collective movement of dislocations, in response of their mutual interactions, external applied loading and interactions with boundaries such as free surfaces, interfaces or grain boundaries. The dislocation microstructures emerging from such dynamics are intrinsically heterogeneous and the way they affect the mechanical properties is a puzzling problem. A reliable tool to model crystal plasticity in micro- and nano-materials is the Discrete-Continuum Model (DCM).

The DCM is based on a coupling between 3D Dislocation Dynamics (DD) simulations and Finite Element (FE) method. In particular, the DD code is in charge of the dislocation microstructure evolution while displacement field and boundary conditions (including surfaces and interfaces) are handled by the FE code. The DCM, which was proposed first in 1999 [1], has been significantly improved during the last years [2]. It is now possible to handle problems with very large number of dislocations when accounting for the influence of complex boundary conditions.

Here, the DCM is used to investigate plastic deformation of Ni micro-samples (in the context of M-ERA.NET project "FASS") and SiGe nanostructures. Those two studies emphasize the DCM strong ability to investigate plasticity in micro- and nano-objects. In addition, the attractive capability of running DD simulations making use anisotropic elasticity is highlighted.

[1] C. Lemarchand, B. Devincre, L. Kubin, J.-L. Chaboche. Multiscale Modelling of Materials, 538 (1999), pp. 63–68

(M5 oral) **Incorporating the nudged elastic band method into dislocation dynamics to investigate thermally activated plastic events**

P-A Geslin[1], Benoit Devincre[2], Riccardo Gatti[2] and David Rodney[1]

[1]Institut Lumière Matière, Université Lyon 1-CNRS, France, [2]Laboratoire d'Etude des Microstructures, Onera/CNRS, France

The study of thermally activated processes is of great importance to understand the evolution of metals and metallic alloys with temperature. The apparition of persistent slip bands (PSBs) in metals deformed under fatigue conditions is technologically important because it eventually initiates material failure. The microstructure of these PSBs and the resulting material properties depend strongly on temperature but the mechanisms in play are still unclear. To investigate this temperature dependent behavior, we have implemented the nudged elastic band method into a dislocation dynamics framework. This method allows to obtain the minimum energy path of dislocation mechanisms within a complex microstructure and deduce the associated activation enthalpy. We consider here in particular the escape of dislocations from a PSB wall, which occurs by bowing out into the channel. This study brings insights into the thermal stability of the PSBs, potentially connected to their evolution with temperature reported experimentally. Moreover, this method can also be applied to study other thermally activated dislocation mechanisms such as dislocation nucleation in complex stress environments.

(M5 oral) **Investigation of plasticity/fatigue mechanisms at interfaces in Ni using ex-situ and in-situ SEM/TEM micro/nano-mechanical testing**

V Samaeeaghmiyoni[1], J Groten[2], H Idrissi[1], R Schwaiger[2] and D Schryvers[1]

[1]University of Antwerp, Belgium, [2]Karlsruhe Institute of Technology, Germany

The goal of this work is to elucidate the fundamental plasticity mechanisms operating at interfaces such as grain boundaries (GBs) and twin boundaries (TBs) during fatigue tests in Ni. To reach this goal, in-situ SEM loading cycles have been performed on single and bi-crystal micropillars with a well-known orientation as revealed by EBSD. Careful characterizations of the nature and the distribution of deformation dislocations, the character and the local structure of the interface as well as the mechanisms controlling the interaction between these defects under cyclic loads were performed using ex-situ TEM techniques including diffraction contrast imaging, HRTEM, nano-strain mapping in TEM as well as electron tomography. In addition, quantified in-situ TEM tensile tests were used in order to directly observe the plasticity mechanisms. In order to minimize the effect of FIB damage on the in-situ experiments, an original method combining twin jet electro-polishing and FIB was used to prepare specimens for in-situ TEM nanomechanical testing.

(M5 oral) **modelling of internal stresses in deformation-induced dislocation microstructures and comparison with experimental data**

M Sauzay and L Dupuy

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The magnitude of the internal stresses generated by dislocation microstructures has been the subject of many controversies [Mughrabi, 1983, Kassner et al., 2013].

The composite model explains the origin of such internal stresses by the plastic strain incompatibilities between soft channels and hard walls. But, the accurate computation of internal stresses in various deformation microstructures is still lacking. Crystal FE computations are then carried out using numerous meshes of PSBs, built based on reported channel & wall widths measured by TEM. The computed mean channel internal stresses range between 10 and 20% of the remote stress, whereas the mean wall ones are about two times the remote stress. The mean phase and stress profiles are in rather fair agreement with the measured ones. Additional discrete dislocation dynamics computations are carried out, modelling PSB walls made of dipolar loops with densities measured experimentally. The internal stresses computed by the FE method and DDD are compared together.

Various other microstructures are considered too [Sauzay, 2008]. The predicted internal stresses in veins/channels are almost negligible but cell backstresses amount to 20% of the remote stress, showing the strong influence of the dislocation microstructure geometry. These results agree well with experimental data [Ungar et al., 1984 & 1991; Levine et al., 2011; Kassner et al., 2013].

The consequences in terms of similitude laws [Sauzay and Kubin, 2011], maximum stable dipole height in walls, and dislocation microstructure formation are highlighted. Finally, close-form expressions are deduced, allowing the proposal of constitutive laws describing crystal kinematic hardening.

(M6 invited) **Predictive metallurgy: from quantum to continuum**

W A Curtin

École Polytechnique Fédérale de Lausanne, Switzerland

The macroscopic performance of metal alloys is now frequently modeled by continuum crystal plasticity. Such an approach captures the preferred slip directions in crystalline materials, but otherwise is a phenomenological representation of the underlying dislocation motion in a complex alloy material. Metallurgical predictions beyond the effects polycrystalline texture requires deeper insights into the mechanisms of dislocation structure and motion, which in turn requires the integrated application of computational and theoretical tools spanning multiple scales. As an example of the predictive power of an integrated approach, we address the problem of the rate- and temperature-dependent flow stress in multicomponent random fcc alloys, which includes the new class of High Entropy Alloys. Multiscale quantum models provide fundamental information on the interaction of individual solute atoms with a dislocation in the material. A theory for the minimum-energy dislocation configuration then leads to predictions for the stress-dependent energy barriers to move a dislocation through the random solute field. Thermal activation theory makes the connection to the rate- and temperature-dependent flow stress. Application of the general theory to successively more complicated problems (dilute fcc metals, dilute hcp basal slip, solute strengthening of twinning in Mg, high entropy alloys) reveals a new level of understanding of flow stress in this class of complex engineering alloys. This approach enables design and/or optimization of alloys, and provides underlying input to crystal plasticity theories. As an example, the role of solutes in influencing dislocation energies is discussed within the context of enhancing ductility of hcp Mg alloys.

(M6 oral) **Flaw insensitivity of defect-scarce nanowires: Atomistic simulations and experiments**

C Brandl[1], C Ensslen[1], G Richter[2], R Schwaiger[1] and O Kraft[1]

[1]Karlsruhe Institute of Technology, Germany, [2]MPI Intelligente Systeme, Germany

The mechanical strength increases with decreasing dimensions of the structure and can eventuelly approach the theoretical strength limit - down to a regime, where the strength of brittle nanostructures is theoretically predicted to be flaw insensitive.

Using atomistic simulations, we investigated the effect of structural flaws, i.e. notches, in intrinsic brittle Si nanowires and intrinsic ductile Au nanowires on the mechanical behaviour. The flaw size and wire diameter dependent strength and ductility in the molecular dynamics (MD) simulations show the existence of the flaw-insensitive size regime. The defect evolution, flow stresses and the strain hardening in the MD simulations of Au nanowires is compared to experimental studies, where gold nanowires were structured by He-ion beams with sub-50 nm notches. The experimental microstructure after deformation - as seen by (high-resolution) transmission electron microscopy - suggests the formation of a nano-grained substructure at the failure location, which is also consistently observed in our MD simulations.

The striking similarities between MD simulations and the experimental data are critically discussed and explained by strain hardening in a strength regime of theoretical shear strength of Au. More generally, the implications of strain rate dependence and temperature dependence of the flow stresses are discussed for defect-free nanowires and its association with thermally-activated dislocation nucleation.

(M6 oral) **MgO nanoparticle deformation at room temperature: insights from MD simulations and in situ TEM**

J Amodeo, I Issa, J Réthoré, L Joly-Pottuz, C Esnouf, J Morthomas, M Perez, J Chevalier and K Masenelli-Varlot

INSA-Lyon, France

Nanocrystalline (NC) ceramics are of particular interest because of their high mechanical characteristics which are better than their conventional counterparts. Thus, NC ceramics are increasingly used as for example in the field of modern orthopaedic surgery where they are employed as femoral heads or acetabular cups, in replacement of metallic alloys. In this context, one way to enhance the mechanical properties of post-processed NC ceramics is to improve our global understanding of the mechanics of ceramic nanoparticles (NPs). Here we investigate the mechanical behaviour of <100>-oriented MgO nanocubes using molecular dynamics (MD) simulations and *in situ* TEM compression tests at room temperature. Results show high strength and ductility, in addition to specific deformation mechanisms interpreted by the simulation. The nucleation and the propagation of ½<110>{110} dislocations are at the onset of the plastic deformation. The different deformation processes as well as the possible formation of a dislocation network during compression are discussed.

(M6 oral) **Multiscale description of the formation of spatially self-confined quasi-one-dimensional nano-phases around dislocations**

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Recent atom probe tomography experiments revealed that chemical and structural nano-sized phases can exist at dislocations in Fe-Mn alloys [1]. These one-dimensional complexion states are fcc in a bcc matrix, characterized by high Mn content and are observed to be self-confined in size, i.e. to be stable against coarsening. A theoretical description of these defects and their energetics is challenging, since they intrinsically couple various mechanisms and structures such as e.g. the dislocation and its strain-field, different phases and the interface between them. To address this challenge we have developed based on our previously developed methodology [2] a computationally highly efficient multiscale approach that describes the formation of these localized states and that combines ab initio calculations with empirical potentials and theoretical mechanics concepts. Specifically, we use atomistic calculations to inform a continuum model based on Eshelby's inclusion. The local elastic field around the dislocation is determined using a semi-empirical embedded atom (EAM) method, and the change in formation energy due to the phase transformation is determined using ab-initio calculations. Using this approach we derive the conditions under which local phase transformation can occur around the dislocation due to its stress field. Our results intuitively explain why quasi-one-dimensional defect can have an equilibrium size and why they become stable against coarsening.

[1] Kuzima M, Herbig M, Ponge D, Sandlöbes S and Raabe D. Science 2015; 349: 1080-1083
[2] Leyson GPM, Grabowski B, Neugebauer J. Acta Materialia 2015; 89: 50–59

(M6 oral) **Solute interaction with the bcc-fcc interface in iron**

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The interaction of alloying elements in solution with the bcc-fcc interface significantly determines the phase transformation kinetics from austenite (fcc) to ferrite (bcc) and resulting properties in low alloyed steels. Computational tools are increasingly used to design and evaluate steel chemistries and industrial processing routes. Typically, the solute-interface interaction is incorporated into these process models in an empirical way by for example adopting an effective interface mobility. To develop models with a more fundamental approach it is critical to account for the atomistic mechanisms of the solute-interface interaction. Here, first principle density functional theory (DFT) simulations are presented for the binding energy of selected alloying elements X (X= Mn, Ni, Cr, Si, Mo) to a bcc-fcc interface. The DFT simulation results are compared to 3D atom probe tomography studies of segregation of these elements to the bcc-fcc in ternary Fe-C-X alloys. The trends of the observed segregation behaviour are consistent with those for the binding energies obtained with DFT simulations. For the investigated solutes, Mo has the largest binding energy and highest segregation level while Ni is the element with the least tendency to interact with the interface. The effect of carbon on solute-interface interaction will be discussed. An outlook will be provided for incorporating these atomistic data into overall phase transformation models.

(M7 invited) **Analysis of experimental grain scale data in a crystal plasticity framework**

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Three-dimensional X-ray diffraction microscopy (3DXRD) has been employed to investigate the behaviour of individual grains deeply embedded in the bulk of interstitial-free (bcc) and austenitic stainless (fcc) steels during tensile deformation. Three-dimensional grain maps have been constructed, meaning that each individual grain is characterised with respect to crystallographic orientation, size and shape. The behaviour of selected individual grains is characterised and their lattice rotations and developing orientation spread are analysed in terms of slip systems by means of crystal plasticity. The differences between individual grains of initially similar orientation will be analysed in relation to their environment of neighbouring grains. The goal is to identify the interaction mechanisms and employ these in prediction of the behaviour of individual grains.

(M7 oral) **Investigation of nonmetallic inclusion-driven failures**

D Naragani[1], M Sangid[1], P Shade[2], J Schuren[2], H Sharma[3], J-S Park[3], P Kenesei[3], J Bernier[4] and T Turner[2]

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Crack initiation at inclusions is a dominant, life limiting and unavoidable failure mechanism as fatigue progresses to find the 'weakest link' in the material to nucleate a crack. It is critical to identify a microstructurally informed driving force to characterize this failure mode. Experiments have been conducted on a Ni-based superalloy sample, produced via powder metallurgy with a seeded non-metallic inclusion, under cyclic loading. The test was sequentially interrupted to conduct absorption contrast tomography to determine spatial and morphological information about the inclusion. Scans were conducted at maximum load to identify the moment of crack initiation and its location in the bulk. High energy x-ray diffraction microscopy was carried out to simultaneously characterize the microstructure surrounding the inclusion. Far field configuration was employed to determine the centroid position, average orientation and stress state of the grains intermittently until crack initiation. Near field setup was utilized to determine detailed spatial information in the form of orientation spread and morphology of the grains and the position of grain boundaries particularly at the crack tip. The reconstructions elucidate temporal and spatial strain evolution of grains in the bulk of the sample especially around the initiation site. Strain localization and the associated stress heterogeneity contain crucial information regarding damage evolution and accumulation; we intend to use this information to determine the driving force for crack initiation for an inclusion driven failure.

(M7 oral) **Towards an experimentally informed multiscale model of FIB-induced irradiation damage**

J Guénolé[1], D Courty[2], E Salvati[3], T Sui[3], R Spolenak[2], A M Korsunsky[3] and E Bitzek[1]

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Over the last decade, focused ion beam (FIB) machining has become a widely used technique in the material science community, in particular with respect to micro- and nano-mechanical testing. Recently, it was proposed to measure intrinsic stresses by FIB-milling of specific geometries and determining the resulting strain relaxation by digital image correlation (DIC) [Korsunsky *et al.*, Materials Letters 63]. Irradiation induced defects are known to influence the properties of the milled samples, depending amongst others on the material, the ion type and energy, and the angle of incidence. This influence on the strain release has yet to be studied in detail. The concept of eigenstrain has been successfully used in higher scale models to predict this effect [Salvati *et al.*, Materials & Design 92]. Recent report of residual stress profiling at the resolution of ~50nm represents an important advance [R. Treml *et al.*, Acta Materialia 103]. However, a further order of magnitude improvement is needed to resolve the stress profile induced by ion beam damage. At present this resolution may only be achieved with the help of numerical models.

Here we present a combined modeling-experimental study of the FIB induced damage in silicon. Detailed atomistic simulations of ion irradiation of atom-probe tomography (APT) needles are performed. The results are compared to careful FIB-implantation experiments analyzed by APT. The ion implantation and induced damage are characterized in detail and the induced strain is determined. The formalism of eigenstrains is used to model the effect of FIB processing on the FIB-DIC procedure.

(M7 oral) **Combined molecular dynamics/experimental study of the strength of Cu|Au multilayer nanopillar systems**

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We used molecular dynamics (MD) to study Cu|Au multilayer nanopillars with 5 nm layer width with (111) cube-on-cube interfaces. We find that Cu|Au multilayers form a semi-coherent interface with a network of partial dislocations arranged in a regular triangular pattern that is susceptible to easy shear. Compression simulations are then carried out at strain rates of 10^8 s^{-1} to study the influence of the angle θ between the (111) interfaces and pillar axis on the interface strength, with θ ranging from 0° to 20°. We find that in most cases deformation occurs predominantly in the softer layer and by sliding along the interface between the layers. For some of the rotation angles we find shear bands that evolve along (111) planes transversal to the semi-coherent interfaces and carry most of the deformation. The stress-strain curve shows a yield stress significantly higher than experimental values and strain softening not observed in experiments experiments. The yield strength is reduced by introducing defects (screw dislocations) into the nanopillar simulations, indicating that the origin of high yield and strain softening is the suppression of dislocation nucleation in defect-free molecular dynamics simulations. The yield strength of the defective nanopillar system is in good agreement with experimental results.

(P2.62) **Dislocation annihilation and sources in continuum dislocation dynamics**

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The dynamics of dislocations as curved line like objects depends on their orientation and curvature. A full representation of dislocation orientation and curvature is given by the higher dimensional dislocation orientation distribution function (DODF).

In Continuum Dislocation Dynamics (CDD) theory, the DODF is represented by a series of harmonic moments called symmetric alignment tensors. The evolution of these tensors describes the glide motion of curved dislocation lines in a density-based setting. Using DODF moments instead of the full function reduces the computational cost tremendously while it allows to capture many important features of the microstructure such as GND and SSD densities and the associated orientations and curvature. However determining the rate of strongly orientation dependent mechanisms such as dislocation annihilation and multiplication needs the access to DODF.

In this paper we apply the 'Maximum Information Entropy Principle' (MIEP) to reconstruct the DODF from the CDD alignment tensors. The resulting approximate DODF is used to evaluate the rates of dislocation annihilation and multiplication and thus to incorporate these processes into CDD. Later we use CDD to investigate the role of dipole formation, dislocation annihilation and multiplication in view of the emergence of dislocation patterns in cyclic deformation of face-centered cubic metals.

(P2.63) **Effect of microstructure on strain localization in Al 7050 Aluminum alloy: modelling deformation using CP-FFT**

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Aluminum alloys still are the preferred material for aircraft's primary structures in aviation. The majority of the load carrying components and fatigue critical locations are made of this material. We seek to understand the mechanical behaviour of AL7050, particularly the strain fields, by means of Crystal Plasticity Fast Fourier Transform (CP-FFT) formulation and experimental mappings. First, the microstructure of rolled Al7050-T7451 was characterized in various orientations with respect to the rolling direction (TL-LT-TS), in order to create microstructure realizations via Dream3D and Matlab. These simulations were subjected to the same loading regime as their experimental counterpart (uniaxial tension and release) via the CP-FFT formulation. The simulated residual strain fields were compared to the fields found on the specimens via Digital Image Correlation (DIC). The results showed that the strain concentrations predicted by the simulation were reasonable for all cases and were statistically representative, however the spatial match needs improvement. Subsequent studies started using columnar Al7050-T7451 specimens and some models also considered the presence of precipitates in the microstructure. With these considerations the simulations have demonstrated improved matches that will facilitate a better understanding of the mechanical behaviour inside the material with future directions leading to the influence of the microstructural features on corrosion pitting.

(P2.64) **Analyzing the effects of powder and post processing on porosity in EBM Ti-6Al-4V**

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To examine the contribution of powder porosity on the final defect population, synchrotron x-ray micro-computed tomography (CT) was performed on the powder, an as-built sample, and a hot isostatic pressed (HIP) sample of Ti-6Al-4V produced via electron beam melting. Initial porosity distributions in the powder were comparable to that of the as built condition. The benefit of synchrotron CT is that is allows a spatial resolution of approximately 1.5 microns, which was able to capture the small pores present after HIPing. Following HIPing, the sample underwent beta annealing, and pore regrowth was observed. To investigate the role of porosity on material performance, elasto-viscoplastic simulations were performed based on fast Fourier transforms. The results demonstrate the role of porosity in the HIPed material acting as hot spots for stress concentration.

(P2.65) **Multiscale modeling of uranium at high pressures**

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Atomistic modeling is widely used to study properties of materials at extreme conditions that are difficult or even impossible to examine experimentally. Published phase diagram of uranium is known only up to 100 GPa. Thus, the melting curve at higher pressures could only be estimated by some kind of extrapolation.

Quantum simulations using density functional theory (DFT) per se are of great numerical complexity. Applying this technique to actinides makes the problem even more complicated compared to other materials: 14 electrons (in case of uranium) per ion are to be taking into account. Thus only small-scaled systems could be calculated. We present a multiscale approach: EAM interatomic potential is constructed based on the DFT data at high pressures and temperatures. Afterwards classical molecular dynamics modeling is performed.

We study a phase diagram of uranium up to 1 TPa and 20 kK by means of quantum and classical molecular dynamics. Modified Z method is used to obtain the melting curve more accurate. Larger spatial scales allow to perform two-phase method (phase co-existence method). Obtained results are in good agreement with experimental data known up to 0.1 TPa and estimations based on DFT results and semi-empirical Simon law.

(P2.66) **Virtual screening process on the precursor development using molecular dynamics simulation**

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This research describes the effective way to find the optimized metal-organic molecules for PECVD precursors. For this purpose, a simple molecular modelling process and easy interface for material engineers was proposed. By using this process, the effectiveness of the candidate materials for the PECVD process could be evaluated before experiments by predicting the basic properties of precursors. Among them, since the vapor pressure of the precursor according to temperature is the most important one to find the effectiveness of the materials, in this simulation process, the force field of the metal-organic molecules were modified to establish the correlated relation on the vapor pressure. Then, for the convenience of the material engineer, the user-friendly GUI would be developed to include the simulation and reporting process for the real application.

(P2.67) **Dislocation patterning and formation of persistent slip bands**

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Work hardening during plastic deformation of crystalline solids is associated with significant changes in dislocation microstructure. The increase in dislocation density on the specimen scale is accompanied by a spontaneous emergence of regions of low dislocation density and clusters of high density which to a large extent persist upon unloading. These *dislocation patterns* (e.g. cell or labyrinth structures, dislocation accumulation in veins or walls) are characterized by fairly universal scaling relationships, commonly referred to as similitude principle. Despite long-standing efforts in the materials science and physics of defects communities, there is no general consensus regarding the physical mechanism leading to formation of dislocation patterns.

We present results from a continuum theory capturing the coupled dynamics of statistically stored and geometrically necessary dislocations while accounting for the specific kinematics of curved dislocations [1]. A surprisingly minimalistic set of 'ingredients' is already sufficient to create patterns that are automatically consistent with the similitude principle. Our simulations explain how cell structures matching experimentally observed structures form. We then demonstrate how data from dedicated discrete dislocation dynamics simulations can be extracted and used for gauging and parametrizing continuum models (e.g. in terms of cross hardening, dislocation sources and annihilation). Together with the mechanisms for dislocation pattern formation, we will show that those are important ingredients on our way towards modelling the formation of persistent slip bands under cyclic loading conditions.

[1] S. Sandfeld and M. Zaiser, Pattern formation in a minimal model of continuum dislocation plasticity, Model. Simul. Mater. Sci. Eng. (6)23

(P2.68) **Multi-scale study of the effect of impurities on oxygen solubility in nickel**

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The fundamental understanding of the oxygen dissolution and diffusion in metals is crucial to understand and predict their behaviour in oxidant atmospheres. Experimental observations suggest that some interstitial species, in particular carbon or hydrogen, could modify oxygen permeability in nickel-based alloys [1]. We present in this poster a multi-scale approach (coupling first-principles calculations and a statistical approach) of the oxygen solubility taking into account interactions with others interstitials species and defects (vacancies) in nickel.

First, DFT calculations were performed to study and to compute the formation and segregation energies of small clusters made of vacancies (V), O, C and H atoms, located either in octahedral or tetrahedral positions. Most stable configurations are presented and analysed. We show for example, that VX clusters (where X=O, H) have strong negative segregation energies. From these DFT results, we have extracted a set of pair interaction energies (X1-X2) according to the X1-X2 distance and the sites.

Finally, we discuss the impact of the V, C, H, O interactions on equilibrium concentration of each defect using a statistical approach based on these DFT parameters.

[1] "Experimental study of the interactions between oxidation and structural defects", S. Pérusin et al., Materials Science Forum vol. 461 (2004)

(P2.69) **Cyclic deformation of Ni micro-pillars with defined crystal orientation at grain boundaries**

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The deformation and failure of polycrystalline metals is directly related to the motion of dislocations and their interaction with grain boundaries, cracks and surfaces. In order to develop fatigue-resistant microstructures a fundamental understanding of these interactions is required. In this study, single- and bi-crystalline Ni pillars of defined orientation were investigated. The micro-pillars were deformed with up to 100 load-unload cycles to study the influence of the GB on the plastic deformation and microstructural evolution. The pillars were prepared by focused ion beam at selected GBs as well as in the adjacent single crystalline regions. The crystal orientation of the grains was characterized by electron backscatter diffraction prior to pillar preparation. Both ex situ and in situ experiments in a scanning electron microscope were performed. Digital image correlation is used to observe the strain distribution and its changes for increasing number of loading cycles. The deformed pillars were carefully characterized using scanning and transmission electron microscopy. Activated slip planes as well as the influence of the grain boundaries on the pillar strength and cyclic deformation behavior will be described.

(P2.70) **Structural determination and electronic properties of one-dimensional Te crystals encapsulated inside carbon nanotubes**

P V C Medeiros[1], S Marks[2], A Vasylenko[2], J Wynn[1], D Quigley[2], J Sloan[2] and A Morris[1]

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We use the ab initio random structure searching (AIRSS) method to determine the geometries of one-dimensional (1D) nanowires formed by encapsulating Te atoms inside single-walled carbon nanotubes (SWCNT). Particular attention is given to narrow SWCNTs (NSWCNTs) with diameters between 5 and 11 Å, since chemical interactions between such NSWCNTs and the encapsulated Te atoms are, in principle, more likely to occur than in SWCNTs with larger diameters. We show that there is a clear preference for the confined Te atoms to form 1D nanowires with helical symmetry. Also, despite the small diameters of the NSWCNTs studied, we show that chemical interactions between the encapsulated nanowires and the NSWCNTs do not play a crucial role in determining the geometries of the most energetically favourable structures. The calculated structural parameters of the encapsulated nanowires are in excellent agreement with the structures synthesised in our experiments. A comparison between our theoretically predicted and experimentally measured electronic and spectroscopic properties shows that our combined theoretical-experimental approach allows for a very precise characterisation of such systems.

(P2.71) **Identifying the microstructurally-short crack growth driving force: combining tomography results, crystal plasticity simulations, and machine learning**

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Identifying the microstructurally-short crack growth (MSCG) driving force for polycrystalline alloys is a critical need in assessing performances of engineering materials subject to fatigue load and to improve both material design and component life predictions. However, due to (i) the lack of “cycle-by-cycle” experimental data, (ii) the complexity of the MSCG phenomenon, and (iii) the incomplete physics of constitutive relationships, only simple damage metrics have been postulated to describe fatigue behavior at the mesoscale level. These damage metrics have been used, in a qualitative and statistical fashion, to compare performances of different microstructures realizations subject to fatigue, but have limited success in predicting MSCG.

Based on experimental results by Ludwig, Guilhem, et al., “cycle-by-cycle” data of MSCG through a beta-metastable titanium alloy (VST-55531) are available via phase and diffraction contrast tomography. These results serve as an input for FFT-based crystal plasticity simulations, in order to obtain the micromechanical fields induced by the presence of the growing crack which compliment the information available from the experiment. Utilizing Bayesian networks, we compute correlations between postulated damage metrics and experimental data. Moreover, experimental and numerical data are combined within a Bayesian machine learning framework, in order to assess the most relevant parameters hidden within the data. This is required to accurately predict the complex MSCG through a postulated damage metric. Work in this area is still on going, in this presentation we will show the framework and preliminary results.

(P2.72) Continuum constitutive law for flexoelectricity in carbon nanotubes from molecular dynamics

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The final aim of this study is to link the multiphysics continuum constitutive laws of Nano-Electro-Mechanical Systems (or NEMS) with the interaction energy between 2 atoms and with their configuration at the atomic scale. At first, the non-linear mechanical behaviour of carbon nanotubes submitted to an external electric field is studied in order to determine its flexoelectric coefficients.

In this communication, we show how the formalism developed in [1] can be extended to the analytic derivation of the "electric" part of the elasticity tensor and include the effect not only of effective dipoles but also of effective charges for a finite population of atoms. We also discuss how to obtain the macroscopic electric field from the molecular dynamics computation. The macroscopic variables such as the strain tensor, the strain gradient tensor and the polarization vector are introduced from the definition of an Elementary Volume representative of the continuum. From these preliminary works, we discuss how molecular dynamics computations can be used to identify the macroscopic responses of a nanotube subject to electromechanical solicitations. More specifically, we show how its flexoelectric behaviour at the continuum scale can be deduced from the study of its mechanical response to an external electric field.

This work was carried out thanks to the help of the “région de Franche-Comté” (grants 2014C-15451 & 2014C-15473). The authors acknowledge useful discussions with Harold Park and Zhao Wang.

[1] H. S. Park, M. Devel, Z. Wang, Comput. Methods Appl. Mech. Engrg., 200, 2447–2457 (2011).

(P2.73) Trapping of H and He atoms at dislocations in tungsten

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Retention of plasma gas components such as hydrogen (H) isotopes and helium (He) is one of the limiting factors in selection of plasma facing materials for future thermonuclear fusion devices. Tungsten (W) is one of the promising candidates for such materials and was chosen for the divertor armor for International Thermonuclear Experimental Reactor (ITER) and as the first wall material for design of demonstrational fusion power plant – DEMO. During the runtime of the thermonuclear installation, such materials undergo the exposure to plasma components, such as isotopes of helium and hydrogen. Although the majority of these elements is released back from the material, a certain amount of them is stored in the subsurface region which inevitably weakens the strength of the considered components.

The latest experiments of retention of plasma components in tungsten at the temperature below 500 K have pointed to the significant amount of retained helium and hydrogen. The latter, unlike helium, does not agglomerate in the form of clusters in the bulk defect-free material. While the low temperature in the experiments excludes the influence of thermally activated vacancies, the lattice defects such as dislocations and grain boundaries are considered as possible traps for hydrogen and helium.

Within the current work the following scientific objectives are addressed: (i) assess and rationalize the binding of H and He atoms to dislocations in tungsten; (ii) provide parameterization for coarse grain models to account for accommodation and detrapping of H and He isotopes from the considered lattice defects.

(P2.74) **Evaluating the contributions to cluster strengthening in aluminum alloys**

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Upon low temperature aging of some aluminum alloys an increase in strength is observed, this increase being as much as 70% of the peak strength in some precipitation hardenable systems. This strengthening, which precedes the formation of GP or GPB zones, is commonly referred to as “cluster hardening” owing to the decomposition of the super saturated solid solution into a non-random arrangement of solute atoms. Phenomenological models for such cluster hardening have previously considered three possible mechanisms: 1) elastic interaction between solute clusters and dislocations 2) di-elastic effects due to solute induced changes in bulk properties and 3) ‘order strengthening’ arising from the change in atomic topology as a dislocation cuts a cluster. In this study we have used atomic scale simulations in an attempt to evaluate the relative importance of these three contributions to the flow stress of cluster hardened binary Al-Mg alloys. The overall results are in good qualitative agreement with the weak cluster hardening of this binary alloy while the relative importance of the three above contributions are different from those typically assumed in phenomenological models.

(P2.75) **Elastic properties of TiN, ZrN and TiZrN thin films sputter-deposited on MgO and Si substrates: Thin film growth and first-principles calculations**

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Transition metal nitrides have been extensively studied, owing to their excellent performance. For most of the applications, thermal stability and elastic properties are of great interest to deal with the durability of the material under service. Several alloys have been proposed in order to improve their properties. Among them, the ternary alloy TiAlN is widely used. Many other transition metal elements can be added to design new properties of nitrides coatings. Assessing the elastic properties of polycrystalline multinary alloys remains challenging as they relate on many attributes: the phase composition, texture, defects. Strategies should be employed to tackle this challenge by studying systems of increasing degree of complexity. This is the aim of the present work dedicated to binary and pseudo-binary cubic single-crystal or polycrystalline TiN-ZrN nitride thin films. They were deposited by magnetron sputtering under reactive Ar+N_2 plasma discharges on a MgO(001), (110), (111) or Si(001) oriented substrates. The elastic constants of thin films can be accurately studied by the Brillouin light scattering and the picosecond ultrasonics techniques which allow measuring sound velocity of surface acoustic waves and of the bulk longitudinal wave that are travelling along the crystallographic direction perpendicular to the film plane. We used this combination to measure the single crystal elastic constants C_{11}, C_{12} and C_{44} and the effectives ones, $\langle C_{33} \rangle$ and $\langle C_{44} \rangle$, of the polycrystalline films. These results are compared to VASP ab initio calculations using the SQS method to mimic the disordered TiZrN alloys, and the self-consistent micromechanical model to evaluate <Cijs>.

(P2.76) **Structural and elastic properties of cathodic arc evaporated TiAlN coatings on WC substrates: experimental and theoretical investigations**

P Djemia[1], L Belliard[2], F Tetard[3], G Abadias[4], Q M Hu[5], C-HLi[3], F Wang[6], F Tasnadi[6] and M J Jõesaar[6]

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Transition metal nitrides coatings have been extensively studied, owing to their excellent performance. For most of the applications, thermal stability and elastic properties are of great interest to deal with the durability of the material under service. Among them, the ternary polycrystalline alloy TiAlN is widely used and studied. Assessing the elastic properties of polycrystalline multinary alloys remains challenging as they relate on many attributes: the phase composition, texture, defects. This is the aim of the present work dedicated to experimental and theoretical investigations of polycrystalline TiN-AlN nitride coatings. Two batches of coatings (500 nm and 2000 nm) were deposited on rotated WC:Co polished substrates at 450°C by cathodic arc evaporation under 4.5 Pa N_2 pressure, using 150 A arc current and three targets A – $Ti_{0.33}Al_{0.67}$, B – $Ti_{0.45}Al_{0.55}$, C – Ti. Well (001)-textured grains with B1-rocksalt structure are characterized by x-ray diffraction while the mass density by x-ray reflectivity. The elastic constants of thin films can be accurately studied by the Brillouin light scattering and the picosecond ultrasonics techniques which allow measuring sound velocity of surface acoustic waves and of the bulk longitudinal wave that are travelling along the crystallographic direction perpendicular to the film plane. We used this combination, together with the conventional nanoindentation technique to measure their effective elastic constants, $<C_{33}>$ and $<C_{44}>$, their Young's modulus and their hardness. These results are compared to VASP ab initio calculations using the SQS method to mimic the disordered TiAlN alloys, and the self-consistent micromechanical model to evaluate <Cijs>.

(P2.77) **Crack propagation modelling for liquid metal embrittlement at the microstructure level**

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Liquid metal embrittlement (LME) is the transition from ductile to brittle fracture when a metallic material is stressed in contact with a liquid metal. After decades of studies, either by macro-scale experiments or by atomic scale grain boundary (GB) characterization, this phenomenon is still fundamentally not well understood.

Experimentally, the LME crack path issue has been recently clarified for steels by nano-scale characterization tools (FIB and TEM) while a classical fractographic analysis fails to provide useful information. Advanced orientation mapping techniques (transmission EBSD and ACOM TEM) were applied. The main finding is that most of the cracking process takes place at grain boundaries, lath boundaries in martensitic steels or mechanical twins in austenitic steels.

The mechanics of LME crack propagation is rarely the focus of study and so far tools able to analyze these environmental fracture cases are lacking in this field. Here, we propose to study LME crack propagation at the microstructure scale, within a crystal plasticity framework used to model plastic deformation in metals and alloys. The microstructure used is either extracted from experimental measurements by 3D-EBSD (Electron Back Scattering Diffraction) or simulated starting from a Voronoï approach. We will show preliminary results of grain boundary crack propagation in such a framework. This approach is undertaken with the goal to be coupled with atomic scale fracture criteria suitable for LME.

(P2.78) **A physical-based approach to study microstructure evolution during production of aluminium semi-finished products**

E Kabliman

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The microstructure evolution undergoing deformation and heat treatment is quite a complex process which requires understanding of underlying mechanisms on different scale levels. In present work a physical-based model developed for simulation of the microstructure evolution (herein recrystallization and grain growth) during manufacturing of aluminum semi-finished products is presented. The model is based on evolution of mean dislocation density and includes information about material properties at different scale levels, from quantum mechanical level (electronic structure), to mesoscale level (precipitation kinetics) and up to continuum level (production and reduction of dislocations). Going further up into macroscale level, real compression tests (with subsequent heat treatment) can be simulated by coupling the model with a finite elements method. At each modeling level the corresponding simulation techniques are employed (WIEN2k, MatCalc, DEFORM™, LS-DYNA, etc.) and supported by various experiments or available literature data. Among those are differential scanning calorimetry, quenching and deformation dilatometer, light and transmission electron microscopy, metallography, electron backscatter diffraction, etc. This enables us to perform a comprehensive study of the microstructure evolution in the aluminium alloys and to integrate the knowledge from small scale models into simulation of the real production process such as rolling or extrusion [1-4].

[1] Materials Science Forum Vol. 765 (2013); p. 429-433
[2] Tagungsband 8. Ranshofener Leichtmetalltage, Geinberg (2014); p. 50-59
[3] Materials Science Forum Vols. 794-796 (2014); p. 728-733
[4] AMAG AluReport Vol. 01 (2015); p.16-19

Symposium N

(N1 invited) **Rolling, sliding and fretting contact of viscoelastic materials**

D Nelias

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The theory of Hertz provides a very simple and unique solution when the materials in contact are elastic, whatever the kinematics of the bodies in contact is. What happens when at least one of the materials is viscoelastic (VE) is far more complex. First the solution becomes transient for rolling/sliding frictionless contact in viscoelasticity. Second an imposed normal load or imposed normal interference leads to a different solution. Third whereas the Hertz solution for the contact between two bodies of revolution can always be solved as an equivalent problem between an ellipsoid of reduced radii against an half-space, one of them being elastic and the other one rigid, rolling and sliding of a VE ellipsoid lead to different solutions.

The transient and then steady state solutions for 3D rolling/sliding contact involving at least one viscoelastic (VE) material will be first presented. Both frictionless and frictional situation will be analyzed.

The presence of one or several heterogeneous inclusions in a viscoelastic matrix will be then investigated.

The last focus will be on fretting contact when one of the materials is VE. The effect of an oscillatory tangential displacement will be discussed.

(N1 oral) **Modelling viscoelastic reciprocating contacts**

C Putignano[1], G Carbone[1] and D Dini[2]

[1]Politecnico di Bari, Italy, [2]Imperial College London, UK

In modern engineering research, wide research efforts are dedicated to analyze and determine the mechanics and physics of soft viscoelastic materials. The significant convolution marking this topic is related to the strongly time-dependent and usually non-linear constitutive stress-strain relations that govern the response of this class of materials. Further intricacy is added when soft bodies are brought into contact and the problem is exacerbated by the multiscale geometry of the intimately mating surfaces. Indeed, a variety of publications has been dedicated to shed light on the contact mechanics of rough viscoelastic solids; these contributions include analytical numerical and experimental studies.

This paper deals with an issue that, in spite of its crucial importance, has not received the attention it should have deserved: the reciprocating contact of viscoelastic materials, where the relative motion between the contacting bodies is periodically inverted. We develop a Boundary Element Methodology that enables us to determine the contact solution in terms of stresses, strains and hysteresis. Specifically, the explicit solution, in terms of a Fourier series of a suitable Green's function is provided. The formulation can be applied to a variety of problems and, in particular, is fully effective when dealing with real surfaces, whose roughens is characterized by a spectrum covering several orders of magnitude.

(N1 oral) **Multiscale plasticity simulation applied to an experimental scratch test on copper using smooth particle hydrodynamics**

S Leroch, S J Eder, A Pauschitz and A Vernes

AC2T, Austria

Scratching is a complex process which is accompanied by plastic deformation and material detachment. Scratch tests are made to characterize the mechanical properties of a given material or coating. Our scratch experiments were carried out using a recently developed scratch/hardness tester able to operate at up to 1000°C under vacuum conditions and loads of up to 500 N. In parallel to the experiments, simulations of the scratch test were carried out on copper using a smooth particle hydrodynamics (SPH) code for solids. Simulations provide deeper insight so that the process can be better understood and exploited as an advanced characterization method. Moreover, this can aid the identification of failure modes and damage mechanisms encountered in laboratory experiments. The SPH code is very flexible as far as the particle resolution is concerned. Thus, we were able to investigate sample sizes from the microscopic to the macroscopic scale. The simulated scratch geometries are in excellent agreement with experimental ones, which also applies to the scratch hardness, giving a measure for the resistance of the material against the penetrating indenter. Moreover, the smooth particle simulation allows the accurate estimation of the real contact area between the indenter and the substrate. Thus, the SPH-simulations provide a feasible method for studying more complex materials, e.g., coatings.

(N1 oral) **Dislocation microstructure evolution in tribological contacts**

J Gagel, D Weygand and P Gumbsch

Karlsruhe Institute of Technology, Germany

Tribological contact properties of metals are governed by the plastic response of the material. A good understanding of the near surface plastic deformation is needed for any predictive modeling of the contact evolution. Therefore, a three dimensional Discrete Dislocation Dynamics tool [1] was adapted for contact problems with a spherical tip. In a first step, indentation simulations were performed to study the dislocation multiplication underneath a spherical contact. The simulations showed that extended prismatic or helical dislocations structures, which dominate the early stages of indentation in experiments [3], can be formed from preexisting dislocations [2]. In a second step, simulations of sliding spherical tips were performed. These simulations give access to the evolution of the dislocation microstructure underneath the moving contact. The specifics of the stress field of a spherical indenter trap dislocations underneath the moving indenter tip. These dislocations are transported with the indenter until they are blocked by grain boundaries. Grain size, crystallographic orientation of the surface and sliding direction influence the dislocation structure. The trapping and therefore the transport is less efficient if active slip directions and sliding direction differ. This leads also to a change in surface roughness, which is calculated from the microstructure.

[1] D. Weygand, L. Friedman, E. Van der Giessen, A. Needleman, Modeling Simul. Mater. Sci. Eng. 10 (4) (2002) 437
[2] J. Gagel, D. Weygand, P. Gumbsch, to be submitted
[3] S. Graca, P. Carvalho, R. Colaco, J. Phys. D: Appl. Phys. 44 (33) (2011) 335402

(N2 invited) **Adhesion between elastic solids: From single-wavelength roughness to self-affine surfaces**

M Müser

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A traditional approach to describing the mechanical contact between two nominally flat surfaces is the multi-asperity view: surfaces touch microscopically at isolated points in space. In this view, each contact patch is assumed to resemble, to a greater or lesser degree, a Hertzian contact. A natural consequence is that adhesive hysteresis is thought to arise predominantly due to the rupture of individual contact points. In other words, the formation or loss of contact happens at points where the gap of the undeformed surfaces has a local minimum.

In my talk I challenge this view and suggest that not only extrema but also saddle points matter, which are best studied using single-wavelength roughness. Their dynamics, just like that of single asperities, becomes hysteretic if adhesion is short-ranged and thereby contributes substantially to adhesion-induced energy loss. The main mechanisms persist when roughness does not only live on one but on a broad range of wavelengths as is the case for almost any surface.

In addition, I discuss why thin foils adhere much better than thick solids. The frequently made argument that thin foils have a greater contact area than thick solids -- also in the absence of adhesion -- does not appear correct.

(N2 oral) **Cavitation of fluids between heterogeneous slipping-sticking surfaces**

D Savio[1], L Pastewka[2] and P Gumbsch[1,2]

[1]Fraunhofer IWM, Germany, [2]Karlsruhe Institute of Technology, Germany

Slip at surface-fluid interfaces can be used to control fluid flow and reduce friction, which is of great interest for the development of lubricated and nanoscale devices. This phenomenon can be achieved by modifying surface chemistry and roughness, for instance through hydro- or oleophobic coatings.

The present work analyzes the shear flow of a lubricant over a heterogeneous surface patterned into sticking and slipping domains, and discusses its consequences from the nanometer to the macroscopic scales.

We first use Molecular Dynamics simulations to show that slip heterogeneity introduces a pressure-driven flow component in addition to the simple shearing of the fluid. Furthermore, high pressure excursions arise along the shearing direction of the lubricated contact. Such behavior is well reproduced by a simple continuum hydrodynamic model based on the Reynolds equation.

We find that pressure variations increase with the pattern length, surface speed, lubricant viscosity and decreasing contact separation. This implies for realistic contact conditions and longer pattern lengths that slip-induced pressure excursions can exceed atmospheric or the externally applied pressure.

Dynamic cavitation should then occur, and we indeed observe it in our Molecular Dynamics simulations. A stable bubble forms over the slipping domain, opening new possibilities for further analysis of cavitation in steady-state MD simulations. Finally, surface separation is enhanced, which can be exploited in lubricated contacts operating in severe regimes.

(N2 oral) **The application of a molecular-continuum coupling strategy for the modelling of liquid lubricants**

E R Fernandez, E Smith, D Trevelyan, D Heyes and D Dini

Imperial College London, UK

The field of nanotribology has (to date) remained slightly detached from mainstream macro-scale tribology, focusing primarily on specialized nano-scale applications. At the macro- and mesoscopic levels, continuum models are often able to correctly model fluids. However, at smaller scales, continuum models do not consider the atomic nature of matter and can sometimes fail to capture the essential physics. In such cases, explicit molecular models must be employed, for example to model a liquid-solid interface.

The development of a truly multi-scale approach, which spans nano- to macro-scales, is a decisive step forward in understanding engineering tribological interfaces. Hybrid methods[1], where atomistic simulations such as molecular dynamics (MD) and continuum computational fluid dynamics(CFD) inter-operate, offer a solution that combines the strengths of both paradigms.

The aim of this project is to model contact-lubrication problems with a multi-scale simulation methodology. To achieve this, an in-house coupling software (CPL_library [2]) has been used to couple MD (LAMMPS) and CFD software (OpenFOAM). CPL_library implements a well-defined interface to facilitate the communication between two arbitrary MD and CFD codes. This employs a domain decomposition approach with an overlapping region where real time data exchange takes place. The method has been applied to study a parallel flow of n-alkanes in contact with an atomistic surface. A coupled simulation approach allows low shear rates which would not be possible with MD alone and to our knowledge have not yet been explored in the literature.

[1] K.Mohamed, A.Mohamad(2010) MANO,8,3,283–302
[2] www.cpl-library.org

(N2 oral) **Molecular dynamics simulations of iron-oxide lubrication by glycerol/water solutions**

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Luleå University of Technology, Sweden

The aim of tribology is to minimize the wear of components, and power and fuel consumption, in order to improve the effectiveness and life-time of the human's machine parks. This is important not only with regard to the economy, but also to effective resource and waste management. Being 100% natural origin fluid, non-toxic, water miscible, and completely biodegradable, glycerol has been found as a promising material to be used as base fluid for environmentally friendly lubricants.

The results of experimental study indicate that under contact pressures as high as 2 GPa, the friction coefficient of glycerol/water solutions can reach 1/4 value of the friction coefficients measured for traditional oil based lubricants in similar experimental conditions. However, the experimental research performed so far is unable to give any indication of the mechanisms of how glycerol’s friction can be so low.

In order to elucidate and understand the processes leading to such excellent lubricant behavior we perform MD computer simulations of the interaction of two iron-oxide surfaces rubbing against each other with a layer of glycerol/water mixtures in between, at high pressure and temperature conditions.

Preliminary results indicate significant fragmentation of glycerol molecules at the lubricant/metaloxide interface. Created fragments undergo chemical reactions with the reactive surface of iron-oxide, leading to the formation of "protective layer" on its surface. Moreover, single or multiple sliding planes between can be observed in the lubricant during course of simulation. Their occurrence is highly determined by the lubricant's temperature and the relative velocity of moving iron-oxide surfaces.

(N2 oral) **The area of contact for non-adhesive rough surfaces: Comparison between MD and Persson's Model**

S Solhjoo and A I Vakis

University of Groningen, Netherlands

In this work we use classical molecular dynamics (MD), and analytical models to study the real area of contact at the atomic scale as a function of the normal load for fractal rough surfaces. To investigate the breakdown of continuum models at the atomic scale, numerical results are compared to Persson's analytical solution, which is a function of surface roughness and material properties.

We present simulation results of the non-adhesive normal contact between a rigid fractal rough surface and a deformable flat. Different rough surfaces are tested by varying the Hurst exponent, while the size effects are investigated by varying the interface sizes. The RMS roughness and the roll-off frequencies are kept constant to generate comparable rough surfaces. The slopes of the rough surfaces are calculated numerically from the generated blocks.

In the case of classical MD, adhesion is turned off by removing the attractive part of the Lennard-Jones potential; while this is not physical, it is necessary to allow for direct comparison with Persson's model. The apparent contact area in the MD simulations is estimated from the projected area of the contacting atoms normalized with the interface area. The contact is defined between the surfaces using a distance-based criterion.

The results are expected to show good agreement between the analytical and numerical solutions at low pressures, while deviations are expected for large pressures and smaller system sizes. Future work will focus on the effect of adhesion in, both, analytical and numerical models.

(N3 invited) **Tight-binding quantum chemical molecular dynamics simulations on tribochemical reaction dynamics of diamond-like carbon thin films**

M Kubo

Tohoku University, Japan

Diamond-like carbon (DLC) thin films have gained much attention as super-low friction materials for automotive engines, aerospace equipments, etc. The detailed understanding of the tribochemical reactions of the DLC thin films is strongly required for clarifying their super-low friction mechanism and designing more efficient super-low friction materials. Here, classical molecular dynamics simulation was frequently employed to investigate the friction behaviors of the DLC thin films. However, the classical molecular dynamics method cannot simulate the chemical reaction dynamics. Therefore, we developed our original first-principles molecular dynamics simulator "Violet" [1] and tight-binding quantum chemical molecular dynamics simulator "Colors" [2] for the elucidation of the tribochemical reaction dynamics [3,4].

In this conference, we introduce the successful applications of our first-principles molecular dynamics simulator "Violet" and tight-binding quantum chemical molecular dynamics simulator "Colors" to the super-low friction properties of the DLC thin films. Moreover, the wear properties of the DLC thin films were also investigated and discussed. Especially, we clarify the effect of the sp2/sp3 ratio, H- and OH-termination, Si-doping, N-doping, Mo-DTC etc. on the friction and wear properties of the DLC thin films. Those investigations confirm the effectiveness of our simulators for clarifying their tribochemical reaction dynamics and super-low friction mechanism.

[1] T. Shimazaki and M. Kubo, Chem. Phys. Lett., 503 (2011) 316
[2] K. Hayashi, M. Kubo et al., J. Phys. Chem. C, 115 (2011) 22981
[3] K. Hayashi, M. Kubo et al., Faraday Discuss., 156 (2012) 137
[4] S. Bai, M. Kubo et al., RSC Adv., 4 (2014) 33739

(N3 oral) **On the solid lubrication processes of silicon oxide containing hydrogenated amorphous carbon coatings**

J Fontaine[1], K D Koshigan[1], F Mangolini[2], J B McClimon[3] and R W Carpick[3]

[1]Ecole Centrale de Lyon, France, [2]University of Leeds, UK, [3]University of Pennsylvania, USA

Diamond-Like carbon (DLC) coatings are well-established solid lubricants, with many successful applications in industry. Their solid lubrication processes are still not understood, since they combine good wear resistance, due to their high hardness, with low friction behavior, which in contrast implies the formation of an easy-to-shear sliding interface. Furthermore, their widespread use is limited by the high sensitivity of their tribological properties to the sliding environment and their limited thermal stability. Adding other elements to the amorphous carbon structure is one way to overcome this Achilles' Heel. In particular, doping the carbon matrix with silicon and oxygen is known to improve the thermal stability and to decrease the environmental sensitivity of the frictional behavior.

In this work, we considered the tribological behavior of silicon oxide-containing amorphous hydrogenated carbon (a-C:H:Si:O) as a function of the environment, which was varied from high vacuum to varying pressures of H_2, O_2 or H_2O). Regardless of the gas, a minimum pressure, i.e., 1 mBar of H_2O, 10 mBar of O_2, or 50 mBar of H_2, is necessary to obtain low friction and wear. Below these pressures, the friction coefficient quickly attained values around 1, with a transfer from the steel counterface to the coated flat. In contrast, above these threshold pressures, the friction coefficients attained values below 0.1, and a carbon-rich tribofilm was formed on the steel. Based on near-edge X-Ray absorption fine structure spectroscopy and Raman measurements, a simple phenomenological model is proposed to account for these observed behaviors.

(N3 oral) **Mechanochemical breaking of C-C bonds at the tribological interface between diamond and silica**

G Moras[1], A Peguiron[1], M Walter[1], H Uetsuka[2], L Pastewka[3] and M Moseler[1]

[1]Fraunhofer Institute for Mechanics of Materials IWM, Germany, [2]Asahi Diamond Industrial, Japan, [3]Karlsruhe Institute of Technology, Germany

Diamond surfaces can undergo wear when sliding against much softer silica surfaces. This process can lead to the wear of diamond tools during the machining of rocks but can also be harnessed in the chemical mechanical polishing of diamond surfaces. The underlying microscopic mechanisms are however hardly understood and recently proposed atom-by-atom wear processes, which are based on the relative strength of C-C and C-O bonds at the diamond/silica interface, need validation.

We use quantum-mechanical simulations to study the stability of diamond (110) surfaces in sliding contact with amorphous silica and with amorphous silicon. We find that C-Si bonds at the diamond/silicon interface are too weak to damage the diamond surface. Conversely, stronger C-O and C-Si bonds form at the diamond/silica interface. However, their strength is insufficient to cause the breaking of diamond-like C-C bonds during sliding and a "weakening" of the interfacial C-C bonds is necessary to observe damage of the diamond surface. In general, weakened bonds can be a result of surface defects or reconstructions. In the case of the diamond (110) surface no defects are needed. Here, the bonding to silica perturbs the aromatic structure of the terminating carbon zigzag structures, thus inducing a chemical activation of the underlying C-C bonds. The mechanochemical breaking of these weak bonds and the subsequent lifting of C-C-C zigzag units mark the onset of degradation of diamond (110) surfaces. This is in contrast to the silicon/diamond interface, where the higher interfacial bond density renders the diamond surface non-aromatic and diamond-like.

(N3 oral) **Tribochemistry of steel lubrication by graphene**

P Restuccia[1], D Marchetto[1], C Righi[2] and S Valeri[1]

[1]Universita' degli Studi di Modena e Reggio Emilia, Italy, [2]CNR-Institute of Nanoscience, S3 Center, Italy

Recent tribological experiments revealed that graphene is able to lubricate macroscale steel-on-steel sliding contacts very effectively both in dry and humid conditions. This effect has been attributed to a mechanical action of graphene related to its load-carring capacity. Here we provide further insight into the functionality of graphene as lubricant by analysing its tribochemical action. By means of first principles calculations we show that graphene binds strongly to native iron highly reducing its surface energy. Thanks to a passivating effect, the metal surfaces coated by graphene become almost inert and present very low adhesion and shear strength when mated in a sliding contact. We perform pin-on-disc tribology experiments that confirm the friction dependence on the concentration of graphene flakes in the lubricant solution, as predicted by the first principles calculations. Finally, we establish a connection between the tribological and the electronic properties of the interface, which is relevant to understand the fundamental nature of frictional forces.

(N4 invited) **Thermodynamics of the Aubry superlubric-pinned transition in D=2 dimensions**

E Tosatti[1], D Mandelli[2], A Vanossi[3] and N Manini[4]

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In 1D incommensurate crystal sliding, the static friction goes continuously from zero (superlubric phase) to finite (pinned phase) as corrugation increases across the so-called Aubry dynamical phase transition. For two dimensional monolayers in a periodic potential, recent molecular dynamics simulations showed a clear first-order superlubric-pinned transition upon increasing amplitude of the periodic corrugation.[1] This transition might be observable in driven colloid monolayers in an optical lattice, which however operate at room temperature. In order to ascertain the persistence of the 2D superlubric-pinned transition at finite temperature we carried out molecular dynamics simulations using the same colloid monolayer studied in [1] as a test case. Preliminary results show that unlike 1D, the 2D Aubry transition does persist at finite temperature, where the first order phase line bends to the right in the corrugation-temperature plane, signaling a higher entropy of the free sliding, superlubric state. When temperature is large enough, the transition broadens out into a clear crossover. Because the two phases appear to have the same symmetry, it can be expected that the 2D Aubry phase line terminates in a 2D critical point, possibly of the Ising type, at finite temperature.(*) ERC Advanced Grant N. 320796.

[1] D. Mandelli, et al., Phys. Rev. B 92, 134306 (2015)

(N4 oral) **Thermal effects on nanoscale van der Waals adhesion and sliding**

M Rastei, M Wierez-Kien, A Craciun, A Pinon, N Beyer, J-L Gallani and M Rastei

IPCMS, France

We present a combined experimental and theoretical study on the effect of thermal energy on adhesion and sliding in mechanically driven nanoscale contacts. By conducting atomic force microcopy experiments on oxides we show that van der Waals adhesion follows a distribution whose density function is an asymmetric bell-shaped curve revealing a temperature-dependent negative skewness [1]. The sliding forces on the same surfaces unveil a stochastic stick–slip friction with slip events spaced by several nanometers [2]. With increasing temperature both the adhesion and friction significantly decrease. We model our findings by using a modified 2–8 Lennard-Jones interaction potential within the reaction rate theory. Our analyses represent a theoretical framework that allows an evaluation of several parameters relevant for adhesion and friction in van der Waals nanocontacts subjected to mechanical fluctuations. The model explains the formation of sudden jumps in the force curves and provides guidelines for predicting transitions from stick–slip to continuous sliding.

[1] A. V. Pinon, M. Wierez-Kien, A. D. Craciun, N. Beyer, J. L. Gallani, and M. V. Rastei, Phys. Rev. B **93**, 035424 (2016)

[2] A. D. Craciun, J. L. Gallani and M. V. Rastei, Nanotechnology, **27**, 055402 (2016)

(N4 oral) **Viscosity and diffusivity of hydrocarbon lubricants under tribological conditions**

K Falk[1], G Moras[1] and M Moseler[1,2]

[1]Fraunhofer IWM, Germany, [2]University Freiburg, Germany

Lubricants in tribological contacts experience extreme conditions like high temperature and pressure, high shear rates, as well as high confinement, especially in the boundary lubrication regime. Under these extreme conditions, the lubricant properties (in particular the viscosity) can differ considerably from expectations based on empirical extrapolations from normal conditions (for example viscosity-pressure relations like Roelands formula).

In this study, we use molecular dynamics (MD) simulations to calculate the viscosities and self-diffusion coefficients of different tribologically relevant hydrocarbon fluids (molecular weights from 170 to 565 g/mol) under extreme pressure and temperature conditions (up to 10GPa and 500K). Exploiting the access MD simulations provide to atomistic details of the fluid behaviour, we discuss the results within the framework of statistical mechanics, in order to connect viscosity to fundamental microscopic properties. In particular, an analysis based on Cohen and Turnbull's free volume theory shows that both diffusivity and viscosity can be robustly predicted as a function of free volume, and hence, as a function of the fluid density. In addition to extreme p,T conditions, we then consider further factors like high shear rates and the confined geometry of a tribo-contact, and discuss how the free volume approach can help pave the way to a universal viscosity model for lubricants influenced by a combination of all the aforementioned factors.

(N4 oral) **Theoretical modeling and experimental validation of film forming mechanisms under deceleration**

J Cayer-Barrioz, D Mazuyer and A Ernesto

LTDS - CNRS - Ecole Centrale de Lyon, France

Nowadays, mechanical systems such as power train or watch movement tribological contacts are optimized in steady-state conditions for which lubrication mechanisms, and film establishment, are generally well known. However, the lubricant failure or surface damage is mainly governed by the fluctuations of the frictional force or the film thcikness due to these non-steady state working conditions (oscillating, fast change in kinematics for instance).

A simple analytical model in 1D and 2D, supported by experimental measurements, is proposed to predict the evolution of film thickness during deceleration. The film forming mechanisms are identified under these transient conditions and the role of the contact geometry, especially the peripheral extension of the constriction zone in the milliseconds preceding the complete halting of the surfaces, is emphasized.

(N5 invited) **Friction is Fracture: Classical shear cracks drive the onset of frictional motion**

J Fineberg, E Bayart and I Svetlizsky

Hebrew University of Jerusalem, Israel

Frictional processes entail the rupture of the ensemble of discrete contacts defining a frictional interface. There are a variety of views on how best to describe the onset of frictional motion. These range from modeling friction with a single degree of freedom, a 'friction coefficient', to theoretical treatments using dynamic fracture to account for spatial and temporal dynamics along the interface. We investigated the onset of dry and lubricated frictional motion by performing simultaneous high-speed measurements of the real contact area and the strain fields adjacent to the rough interface separating two spatially extended blocks. We show that the transition from static to dynamic sliding is mediated by earthquake-like rupture fronts that propagate along the interface, while dissipating energy by fracturing the discrete contacts along the interface. We demonstrate that the transition from 'static' to 'dynamic' friction is quantitatively described by classical singular solutions for the motion of a rapid shear crack which provide us with a quantitative measurement of the fracture (dissipated) energy at the interface. We find this framework provides quantitative predictions for where the rupture fronts arrest along the interface that are in excellent correspondence to the measured arrest lengths. We then investigate the effects of boundary lubrication and shown that, surprisingly, although reducing the frictional strength of the interface (friction coefficient), lubricants actually significantly *increase* the fracture energy (amount of dissipated energy) during rupture. Thus surface lubrication, while strongly reducing the residual stresses in the wake of rupture propagation, actually *toughens* the contacting surfaces.

(N5 oral) **Molecular modeling of liquid/solid friction for nanofluidic applications**

L Joly[1], G Tocci[2], S Merabia[1] and A Michaelides[3]

[1]Institut Lumière Matière, Université Lyon 1, France, [2]Ecole Polytechnique Fédérale de Lausanne, France, [3]University College London, UK

Nanofluidic systems (i.e. natural and artificial systems where fluids are confined at the nanoscale) play a key role in numerous present-day applications, from water treatment to sustainable energy harvesting. New behaviors arise in nanoconfined liquids due to the dominant role of surfaces. For instance, nanoflows are controlled by interfacial hydrodynamics, and can be enhanced by liquid/solid slip arising from low liquid/solid friction. Electrokinetic effects, coupling different types of transport at interfaces, at the core of nanofluidic energy conversion systems, can also be enhanced by liquid/solid slip. It is therefore crucial to understand and optimize liquid/solid friction in order to design more efficient nanofluidic devices.

During this talk, I will illustrate how molecular dynamics simulations can help unravel the molecular mechanisms underlying liquid/solid friction. In particular, I will present recent work where we used large-scale ab initio molecular dynamics simulations to investigate the coupling between fluidic transport and interfacial chemistry. To that aim, we focused on carbon and boron nitride nanostructures, which offer great promise for nanofluidic applications. We showed that water friction on these two materials is different, although their wetting properties are identical, and that the difference in friction arises from specific electronic structure effects. We then showed the crucial role of defect reactivity in real systems. To conclude my talk, I will discuss how the presented toolbox can be extended to explore the coupling between liquid/solid friction and interfacial chemistry in lubricated contacts, where the system is generally far from equilibrium, with severe mechanical and thermal constraints.

(N5 oral) **Contact mechanics of polymer composites; a decoupled multi-level approach**

L van Breemen, S Krop and H Meijer

Eindhoven University of Technology, Netherlands

Polymers play an increasingly important role in tribological applications. This is a challenging subject because of the complex contact conditions involving many variables. Therefore, simplification to a well-defined contact situation is needed: the single-asperity sliding friction test. With this test, a wide range of surface mechanical properties are analyzed in a controlled manner. In a previous study a hybrid experimental-numerical approach was employed which revealed the subtle interplay between the constant polymer-indenter adhesion and the velocity/rate-dependent deformation of the polymer during scratching [1]. Understanding the polymers' intrinsic mechanical response proved to be key.

In practice, however, most polymers are filled. These fillers are added for many different reasons: to improve mechanical properties, to change the appearance, or even to reduce costs by adding a cheaper material in the polymer matrix. These additives have an effect on both the intrinsic mechanical response, and the adhesive interaction with the indenter tip. Consequently, the frictional response of the polymer changes completely.

To characterize the effect of filler particles experimentally, a thermoplastic model material (polycarbonate) and a thermoset model material (standard epoxy) are filled with either hard (TiO2) or soft (rubber) particles [2]. An identical experimental-numerical approach is used to investigate the response of these model systems. The effect of adding fillers to the polymer matrix is revealed by scratch tests; the interplay between composite-indenter adhesion and the composites' response to deformation are revealed by finite-element simulations.

[1] Van Breemen et al., Wear 2012, 274-275, 238-247
[2] Krop et al., JMPS 2016, 87, 51-64

(N5 oral) **Towards a full picture of a lubricant behavior under severe conditions**

L Martinie[1], S Ndiaye[2], N Fillot[2], D Philippon[2] and P Vergne[2]

[1]INSAVALOR, France, [2]LaMCoS, France

In a highly-loaded lubricated contact, the macroscopic tangential force measured at the solid/lubricant interface displays a plateau at moderate sliding. The corresponding shear stress, called *Limiting Shear Stress* (*LSS*), is representative of a significant change in the lubricant behavior which has already tried to be explained in literature, either by the lubricant microstructure evolution (solidification or shear localization) or by the onset of slip at the interface. Unfortunately, the microscale evidence of this macroscopic behavior is still hardly accessible by dedicated experiments, due to the extreme pressure and confinement conditions. Thus, up to now, *LSS* remains phenomenologically modelled from friction measured in highly pressurized lubricated contacts.

Few atomistic approaches (MD) are emerging to directly get information at the nano / micro scales. They propose a phase diagram of the lubricant, covering wide ranges of pressure and shear velocity, which includes all the scenarios quoted above. However, this approach involves very strong assumptions, among them the use of a Lennard-Jones fluid, and this kind of phase diagram has never been experimentally validated.

This presentation aims at comparing predictions from MD with macroscopic experimental results in order to validate the numerical phase diagram. For this purpose, results obtained over large ranges of pressures and deformation rates from both literature and experimentations performed at LaMCoS are gathered and discussed. This approach, combining MD simulations and experimental work, helps to gain further understanding of the mechanisms behind the concept.

(N5 oral) **Capturing the small and large scales effect when modelling mixed lubrication**

N Brunetiere

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According to the Reynolds lubrication theory, it is not possible to generate any hydrodynamic load in the lubricating fluid between two parallel surfaces. However, when the friction coefficient measured during experiments is plotted as a function of the duty parameter G, a typical Stribeck curve is obtained, indicating that a hydrodynamic force is generated.

Real surfaces are not perfectly flat because of the roughness, explaining thus the load generation. Considering surface roughness in lubrication problems has first been done by stochastic approaches and later by homogenization technics. However, these theories are not able to explain the load generated during experiments. The only solution is to perform a deterministic simulation where a mesh thin enough to capture the local topography of the surfaces is used. However, this method suffers from two main limitations. First, it is limited to small contact area. Secondly, a mesh converged solution could necessitate a very fine mesh. These two problems are addressed in this presentation. In the first part, a multi-scale approach is used to capture the large scale effects. The use of a second macroscopic scale allows increasing the size of the domain and reducing computation time. In the second part, a method inspired from Large Eddy Simulation (LES) used in fluid mechanics is used to capture the effect of the small without increasing the number of nodes. For that the equation are filtered and a sub-grid model based on a stochastic approach is used.

(N6 invited) **An adhesive wear map for rough surfaces in dry sliding contact**

J-F Molinari[1], R Aghababaei[2], G Anciaux[2] and L Frérot[2]

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We present molecular dynamics simulations of dry sliding contact between atomistically rough solids. For the case of a ductile (metallic) model material, we show that roughness is strongly altered during sliding motion. It is evidenced by a surface flattening that follows an exponential decay and quickly reduces friction to almost zero. However, more diverse mechanisms appear if we increase the brittleness of our atomic potential, which can be used to span third-body length scales (defined by the ratio of hardness over surface energy) amenable to MD small system sizes. This allows the exploration of wear processes from single atom removal to debris formation as experienced at engineering scales. We discuss the interplay between microcracks, debris and roughness creation. Our simple model recovers the main features of engineering wear laws and shines new light on why debris formation is a rare process. We then use this knowledge in mesoscale (continuum mechanics) simulations of rough surfaces to predict the dependence of the wear coefficient on the applied normal load, and in particular to shine light on the transition from mild to severe wear.

(N6 oral) **Simulation of dry friction and wear at mesoscale using a multibody approach**

G Mollon

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The third-body concept is often used to describe the thin layer of degraded material which separates contacting bodies during friction. If such phenomena as friction and wear are to be fully understood, an accurate modelling of the third body is hence crucial. In recent years, simulation methods based on Discrete Element Modelling (based on interacting rigid particles) have been successful in understanding several properties of the third-body behavior. The next stage, however, is to render each third-body particle compliant in order to be able to deal with important phenomena such as complex constitutive laws, plasticity, Poisson effect, surface adhesion, etc. A consistent numerical framework for this task is presented in this communication, based on a multibody meshfree method developped for this purpose. The method is first presented, and it is then shown how its features might allow future discoveries about the behavior of third-bodies, and enhance prediction of friction and wear.

(N6 oral) **Thermostatting effects on microstructure evolution and material removal during grinding of a polycrystalline Fe surface - A molecular dynamics analysis**

S J Eder, U Cihak-Bayr, D Bianchi and A Pauschitz

AC2T Research GmbH, Austria

We perform large-scale molecular dynamics simulations of abrasive particles grinding on a rough polycrystalline ferritic surface subject to various modes of thermostatting. We first give an overview of our pre-processing scheme to produce an annealed nanocrystalline substrate microstructure with a realistic grain size and misorientation distribution, followed by a brief description of how we generate the fractal surface texture as well as a random lateral and normal size distribution of multi-faceted hard abrasives. Dry grinding takes place at several constant normal pressures and at a slight angle with the system's coordinate system to minimize artifacts of periodicity. To remove the heat caused by deformation and friction during the process, we employ several variations of a Langevin thermostat acting on different parts of the tribosystem. A time- and pressure-resolved analysis of the temperature distribution, the microstructural changes in the substrate, the surface topography as well as the material removal reveals vast differences between differently thermostatted processes, especially for normal pressures exceeding 500 MPa. We conclude with a discussion of which thermostatting mode most accurately reflects realistic process conditions and give an outlook towards the integration of metal working fluids into the system as an additional means for controlling the temperature of the substrate and the removed material.

(N6 oral) **Lattice defects evolving in subsurface zones during grinding processes of polycrystalline ferritic iron**

U Cihak-Bayr, D Bianchi and S J Eder

AC2T Research GmbH, Austria

Mechanisms of subsurface damage and material removal of polycrystalline ferritic iron are investigated under nanoscale grinding by multiple rigid abrasives with random orientations. In a 3D molecular dynamics simulation model, the iron substrate was set up with a random texture and a rough surface. The random orientation of the abrasives combined with their positions relative to the substrate asperities allows a realistic simulation setup with various indentation depths and rake angles. For different normal pressures, the effect on the subsurface modifications as well as the wear of the substrate are illustrated and quantified. Grain growth due to frictional heat caused by passing abrasives could be observed even in structures that were well annealed prior to grinding. Appreciable evolution of dislocations and mobile grain boundaries were only observed in the first layer of grains. Higher pressure does not seem to increase the dislocation density in all grains but rather enlarge the sheared region as well as the thermally influenced zone beneath a passing abrasive. The crystal structure of this subsurface region is evaluated as a function of time to understand the deformation mechanism in the substrate and the stability of grain boundaries.

(N6 oral) **Effect of the metallic counterface material on tribochemical wear of DLC coatings**

S Lafon-Placette[1], J Fontaine[1], M I De Barros[1] and C Héau[2]

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Diamond-like carbon (DLC) coatings are successful in tribological applications thanks to their low friction and low wear. Many studies have focused on describing their friction behavior in several environments and under different operating conditions. However, their wear mechanism in boundary lubrication and the way they interact with the lubricant and the counterface is still not well understood. The variety of DLC coatings, according to their hydrogen content, carbon hybridization (sp^3/sp^2) or alloying elements, as well as the numerous types of lubricant or counterfaces makes it difficult to determine, from the abundant literature, which combinations are really the most effective. For lubricated applications, the understanding of their wear behavior only in base oil is necessary for proposing optimized lubricant additives.

Preliminary results of this study showed that hardness of the DLC coating does not prevent from wear. Tetrahedral amorphous carbon coating (ta-C) with a high hardness showed higher wear than amorphous hydrogenated carbon coating (a-C:H) when sliding against steel in base oil at 110 °C. An a-C:H coated steel counterface reduced significantly the wear rate of both DLC coatings. This result combined with EDX and XPS analysis suggested that chemistry is involved in wear of the sliding contact and and that iron may promote the formation of a heterogeneous and adherent carbon-based tribofilm on the steel surface. To go further, several metallic coatings were deposited on the steel counterface and tribological experiments revealed that the nature of these metals played a significant role on the wear resistance of the DLC coatings.

(N7 invited) **The impact of coulombic interactions among polar molecules and metal substrates on lubrication properties**

K Gkagkas[1] and V Ponnuchamy[2]

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In our quest for lower energy losses, a deeper understanding of lubrication mechanisms is necessary. Solid-liquid interactions are especially significant. Atomic-scale simulations can provide important insights. For example, Loehle et al. have shown the impact of different fatty acid molecule structures on their lubrication properties.

In the case of polar molecules interacting with metal surfaces, the impact on the surface charge distribution can potentially affect the overall system behaviour. Such interactions can be studied with DFT calculations, however their computational cost renders them impractical for engineering applications. Instead, they can be approximated in MD simulations via the implementation of charge equilibration methods such as QEq. Additionally, many body potentials such as EAM and COMB can be applied to describe metals.

Such schemes have been employed extensively for modelling a wide range of systems including metals, metal oxides and metal-ceramic oxide interfaces. In this study, we evaluate their implementation for the case of metal-liquid interfaces and assess their accuracy against DFT calculations. We quantify the impact of the inclusion of such interactions on bulk system properties such as wetting and shearing behaviour. Such results can form the basis for describing the physico-chemical lubrication mechanisms and guide us in the efficient multi-scale analysis of tribological systems.

As a simplified example, we have calculated the charge distribution inside a Cu lattice covered with alternating layers of Li and Cl, while implementing EAM and LJ potentials for the description of the Cu solid. A significant impact on the solid surface charge was observed.

(N7 oral) **Understanding the tribological behavior of industrial additives in ACH/ACH systems using Tight-Biding Quantum Chemicamethod**

E Deguillard[1], S Loehlé[2], S Bai[3] and M Kubo[3]

[1]Total, Japan, [2]TOTAL Marketing & Services, Centre de Recherche de Solaize, France, [3]Tohoku University, Japan

Diamond-Like-Carbon (DLC) films are amorphous carbon material that include tetrahedral amorphous carbon (ta-C), hydrogenated DLC (a-C:H), tedrahedral hydrogenated amorphous carbon (ta-C:H), and non-hydrogenated DLC (a-C) [1]. Showing excellent tribological properties such as low friction coefficient, hardness, or wear resistance, they are now widely used as coating materials in the automotive industry to extend the lifetime of motor parts or reduce the emission of CO_2. However, DLCs' performance widely depends on the lubricant and additives used [2]. Thus, a lot of studies are on-going to better understand the interactions of DLC with various additives molecules [2] but some effects are yet to be completely understood [3].

Computational methods are a very useful tool when it comes to investigate such systems at an atomistic scale [4]. In this work, we compare, by mean of a tight-binding quantum molecular code [5], the friction behavior at the boundary lubrication conditions of two models of amine-type additive molecules, in an ACH/ACH system under different loads. We show that, due to the composition of the amine molecules and the chemical stability of the ACH, that these additives reduce the friction coefficient by limiting chemical interactions between the DLCs while providing a protecting effect for the DLCs.

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(N7 oral) **Effect of graft density on the wear of polymer brush by coarse-grained molecular dynamics simulation**

R Takakuwa[1], Y Ootani[1], T Nishimatsu[1], Y Higuchi[1], N Ozawa[1], Y Tsujii[2] and M Kubo[1]

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Polymer brush has attracted attention in many areas because of its good frictional properties and biological compatibility. Y. Tsujii *et al.* revealed that concentrated polymer brush realizes better lubrication than semi-dilute polymer brush. However, the wear of brushes is a severe problem. Although understanding the wear mechanism of brushes is essential, it is difficult to experimentally obtain the dynamics of polymer chains in molecular scale. We investigated the wear mechanism of polymer brush and the effect of graft density by our coarse-grained molecular dynamics simulator.

Friction simulations of the low (100 chains/substrate) and high (196 chains/substrate) density models are carried out. During friction at high load, polymer chains are dissociated, which corresponds to the wear. Polymer chains were easily dissociated near the upper substrate and at the friction interface between the upper and lower brushes. Near the upper substrate, some monomers are pushed onto the substrate and pulled by the slid substrate. Other monomers are pulled to the opposite direction. Therefore, the stress is concentrated on the boundary. At the friction interface, the entanglements of the upper and lower brushes were converged and the stress is concentrated. In higher density brush, fewer beads are pushed onto the substrate and the entanglements are fewer at the interface. Thus, the dissociation number of higher density brush is lower at the friction interface and near the upper substrate. We revealed the reason why polymer chains are easily dissociated at the friction interface and near the upper substrate and the effect of graft density.

(N7 oral) **Ionic liquids as lubricants: a multi-parameter and multi-scale puzzle**

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An increasing number of studies points out the potential of ionic liquids as lubricants. This work focus on their behavior in nanoconfinement, using molecular dynamics simulations and some insight is given on how this could affect the contact at the microscale.

At the nanoscale, previous work established the highly important role of the fluid / solid interface on local rheology. In fact the interface topology and the thermal conductance respectively drive the interfacial slip and, through the variation of temperature, the viscosity of the fluid. Based on this analysis, different kinds of actual lubricated surfaces (DLC, oxides) were included to the study to anticipate their response in ionic liquid lubricated systems. The results confirm the compelling influence of the surface type on the nanoconfined rheology.

At the microscale, the integration of a wall slip parameter in the Reynolds equation will contribute to improve the classical numerical models. Therefore, finite element simulations of the ionic liquid confined between different surfaces can be run taking as an input the previously calculated wall slip related to each surface.

(P1.59) **Effect replacement of V BY Nb and Fe on the tribological behaviour of biomedical titanium alloys**

F Mamoun

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Biometallic materials are the most important materials for use in biomedical applications especially in manufacturing a variety of biological artificial replacements in a modern worlds, e.g. hip, knee or shoulder joints, due to their advanced characteristics. Titanium (Ti) and its alloys are used extensively in biomedical applications based on their high specific strength and excellent corrosion and tribological resistance. To overcome the potential V toxicity, V was replaced by Nb and Fe, leading to two new V-free α+β-type Ti-based alloys, i.e., Ti-6Al-7Nb and Ti-5Al-2.5Fe. The purpose of this study is to evaluate the friction and wear behavior of high-strength titanium based alloy.The Oscillating friction and wear tests have been carried out in ambient air under different conditions of normal applied load and sliding speed, as a counter pairs we used the ball of 100Cr. The surface morphology of the titanium alloys have been characterized by SEM, EDAX, micro hardness, roughness analysis measurements.

(P1.60) **Coarse-grained simulations of polyelectrolyte brush interfaces**

T Kinjo, H Yoshida and H Washizu

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Polymer brush has long been one of major topics in polymer physics and chemistry because of its wide applications, such as colloid stabilization, wetting, adhesion, lubrication and so forth. Among them, we are interested in the lubricating properties of the surface between opposing polymer brushes. The purpose of our research is to investigate the mechanism of low friction of the surfaces between polyelectrolyte brushes. In this study, as a first step, we focus on static structures of single and opposing polyelectrolyte brushes. Our model is based on dissipative particle dynamics method. In conventional dissipative particle dynamics method, the interactions between particles are represented by Groot-Warren's soft beads potential. In this study we use Groot-Warren potential for solvent particles and Lennard-Jones potential for polymers and ions. The long range electrostatic interactions are calculated by PPPM method. We investigated the influence of the chain length, grafting density, charge fraction and salt concentration on the structures of polymer layers. We find that mobility of the ion and solvents are higher near the free end of the grafted polymers, and in the interface between opposing brushes, the interpenetrations between brushes are small.

(P1.61) **ReacLub: Strong coupling between flow and physical chemistry in lubricated contacts**

S Tromp[1], N Fillot[1] and L Joly[2]

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One of the major current technological challenges consists in reducing the size, weight and environmental impact of tribological systems. The reduction of the amount of lubricant quantity is nowadays coupled with the use of low-viscosity fluids (e.g. refrigerant), so that the width of lubricating films can reach nanometric scales locally. Specific behaviors at the nanoscale arise from the particular role of surfaces and possible chemical reactions.

Because experimental in-situ analysis inside the contact area is still very difficult, we aim at providing numerical simulations, which enable us to observe the chemical reaction at the interface between the refrigerant and the surface. On one hand, the interfacial dynamics is affected by the physical chemistry of the interface (e.g. chemical reactions), but on the other hand the flow itself can control the chemistry.

The present work focuses on the development of a methodology to analyse with both ab-initio and force fields molecular dynamics the behaviour of a refrigerant in realistic functioning conditions, where the system could be far from the equilibrium. This project is based on the understanding on how the physical chemistry of interfaces and refrigerant flows interact, and in particular how severe flow conditions can trigger or affect structural/chemical changes for the confined liquids and the liquid/solid interfaces.

(P1.62) Study of diffusion and adsorption mechanisms of amine-based friction modifiers using Tight-Binding and Molecular Dynamics simulations

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Since fuel economy is an important economic and environmental issue, friction-modifier additives in automotive lubricants have become a crucial solution to improve efficiency of these engines. In particular, organic friction modifiers are used to improve tribological performance in boundary and mixed lubrication regimes, by forming a protective film on metal surfaces and preventing them from direct contact [1]. Besides, nitrogen-containing compounds (amines, amides and imides) seem to be promising additives due to their sulfur- & phosphorus-free chemical composition. Therefore, they fulfil the environmental requirements of the recent automotive emission legislation, which impose low concentration of SAPS (Sulphated Ash, Phosphorus and Sulphur) in lubricants.

In this computational study, we have investigated the mechanisms of action of amine-based friction modifiers using the *Tight-Binding* and the *Molecular Dynamics* methods. Two important phenomena were studied: the *diffusion* of different fatty amines in a model base oil and their *adsorption* on iron-based surfaces. The aim was to better understand the effect of the chemical structure of the fatty amines on the thermal film formation and eventually on their tribological behaviour.

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(P1.63) Shear response of a fluid under extreme pressure and stress

S N Ndiaye, P David, M Laetitia and V Philippe

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In highly loaded lubricated contacts, the friction coefficient defined as the ratio between tangential and normal forces, displays a plateau for high shear rates or moderate SRR (slide-to-roll-ratio). The corresponding shear stress is known as the so-called Limiting Shear Stress (LSS). The physical origin of the friction plateau is still an open question and is not easy to investigate due to the extreme pressure and confinement conditions occurring in these contacts. Several attempts are proposed in the literature to explain the occurrence of the LSS involving either the solid surfaces / liquid interface or the lubricant microstructure. Nevertheless there is no clear consensus on the mechanisms behind the LSS. Consequently, LSS is empirically predicted to evolve linearly with the contact pressure, which causes a real weakness in the current models of friction in highly-loaded lubricated contacts, as those found in rolling element bearings.

Our research aims at developing a new methodology allowing to simultaneously measure the friction in such contacts and to follow in situ the lubricant microstructure evolution by coupling a ball-on-disk tribometer with a spectroscopic technique.

This approach will help to experimentally identify the nature of the mechanisms behind the LSS, either microstructural or from local phenomena in the interface. This understanding is essential to provide a robust modelling of the LSS phenomenon.

(P1.64) Quantum chemical molecular dynamics simulations for clarifying super-low friction mechanism of carbon nitride thin films

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Carbon nitride (CNx) thin films have gained much attention as solid lubricants for automotive engines, aerospace instruments etc. and have been intensively studied. The previous experiments showed that CNx thin films have lower friction property than diamond-like carbon (DLC) thin films, however this mechanism has not been clarified. Although it is pointed out that the tribochemical reaction is key for the super-low friction property of CNx, the atomistic mechanism of the tribochemical reactions has not been clarified by experiments. In this study, we intend to elucidate the tribochemical reaction dynamics of CNx and its influence on the super-low friction mechanism by our tight-binding quantum chemical molecular dynamics simulator [1-3]. Our simulation results of H-terminated CNx and H-terminated DLC under 1 GPa show low friction coefficient of 0.05. However, H-terminated DLC shows high friction coefficient of 0.43 under 5 GPa. On the other hand, H-terminated CNx shows low friction coefficient of 0.07 even under 5 GPa. Here, many C-C bonds are generated at the H-terminated DLC interface, although C-C and C-N bonds are not generated at the H-terminated CNx interface. Therefore, we conclude that H-terminated CNx films show low friction coefficient than H-terminated DLC films under high pressure because H-terminated CNx films prevent the generation of C-C bonds at the friction interface.

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(P1.65) Multiscale modeling of friction in structured surfaces

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Examples of hierarchical multiscale structures can frequently be found in Nature. This is because significant improvements in the mechanical properties can be induced by variations in structural and geometric arrangements at various size scales rather than by a change in constituent materials with different mechanical properties. Up to now, these effects have been studied in many different fields, such as continuum and fracture mechanics, or for adhesive or super-hydrophobic materials. However, in tribology the effects of multiscale structures in solid-solid interfaces have not yet been fully investigated. Moreover, in the presence of impurities and anisotropies, always present in experiments, the tribological behaviour of real materials is much more complex than at present predicted by theoretical and numerical models.

We present a systematic study using numerical simulations based on statistical models, in order to investigate the friction behaviour in the presence of surfaces with hierarchical structures and anisotropies, such as in the snake ventral scales. Results are compared with FEM simulations on surfaces with different elasticity, anisotropy, and roughness. We show how some characteristic effects due to the complex geometry can be captured by a simplified (and less computationally demanding) model, in which the system is discretised in basic mass-spring or damper elements together with statistical distributions of the elastic and local friction parameters, in order to take into account the spatial, hierarchical, and random variability of interface properties.

(P1.66) **Understanding of the electronic structure and mechanism of linkage isomerization in molybdenum dithiocarbamate**

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Molybdenum dithiocarbamate (MoDTC) is a well-known dinuclear bridged Mo-S complex which is used as a lubricant additives in automotive industry for many years. But the tribochemical reaction pathway of MoDTC to form MoS2 sheets is highly complex and not yet completely understood. It plays an important role in the ageing of the oil. We have used DFT calculations based on the experimental observations for a deeper understanding of the complex interactions that are not accessible by experiments alone. We explored the electronic structure and geometry of MoDTC before and after reduction. We found that 1 ē reduction of MoDTC is necessary for linkage isomerization reaction.

(P1.67) **Development of movable cellular automata for the prediction of friction and wear**

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Tribology is considered a difficult subject due to the complex multi-scale nature of interactions between contacting surfaces. A clear separation of micro and macro-scales is principally impossible in tribological phenomena such as friction and wear, however, there is a lack of coupling between the scales. For reliable predictive models to occur, tribosystems have to be modelled as a whole; the surfaces and the interactions between them. Here, the Movable Cellular Automata (MCA) method is used and developed to model friction and wear processes in three-dimensional nano-indentation scratching tests.

MCA represents a medium as a discontinuous system of particles (or automata); very much like the discrete element methods, however, the interaction between the particles is based on many-body forces of inter-automata interactions; similar to the molecular dynamics method but on larger scales. It is also based on the classical cellular automata method where the interaction between these automata can lead to the change of their state, which is based on a bonding/fracture criterion which is calibrated using experimental nano-indentation tests, and is considered optimal when the numerical and experimental results match.

MCA is feasible on the nano and micro-scales and can effectively simulate the inhomogeneities in material characteristics and plastic deformation, but it is not efficient at the macro-scale,. However, it can be coupled with continuum methods such as the finite elements method. Due to the mobility of the automata and the ability of changing their state, MCA is capable of effectively modelling many material processes including friction and wear.

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